Sample name: **M08_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-02009**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02009_M08_octanol_pH-metric high logP.t3r**

Experiment start time: **3/2/2018 8:29:22 PM**
Analyst: **Pion**
Instrument ID: **T312060**

pH-metric Result

logP (neutral XH)   3.16   ±0.01 (n=50)
logP (X -)   0.23   ±0.03 (n=50)

18C-02009 Points 2 to 38

M08_octanol concentration factor   1.095
Carbonate   0.0863 mM
Acidity error   -0.76941 mM

18C-02009 Points 39 to 63

M08_octanol concentration factor   0.769
Carbonate   0.0001 mM
Acidity error   -0.70585 mM

18C-02009 Points 64 to 92

M08_octanol concentration factor   0.703
Carbonate   0.2882 mM
Acidity error   -0.43720 mM
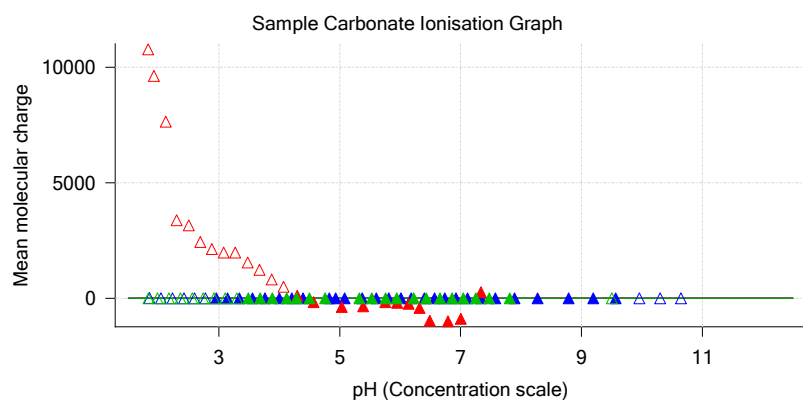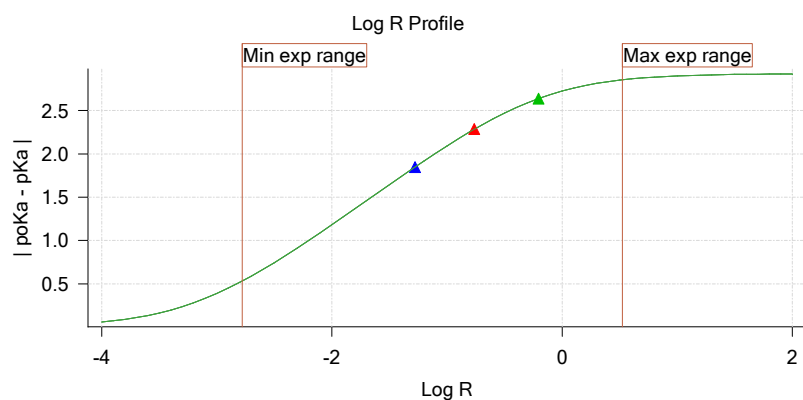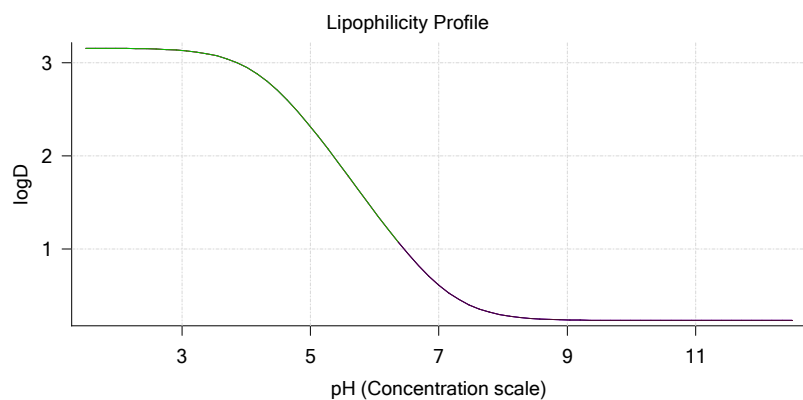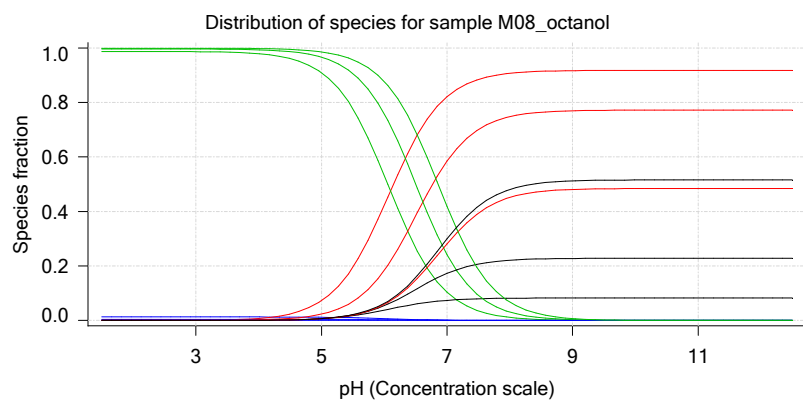
Warnings and errors
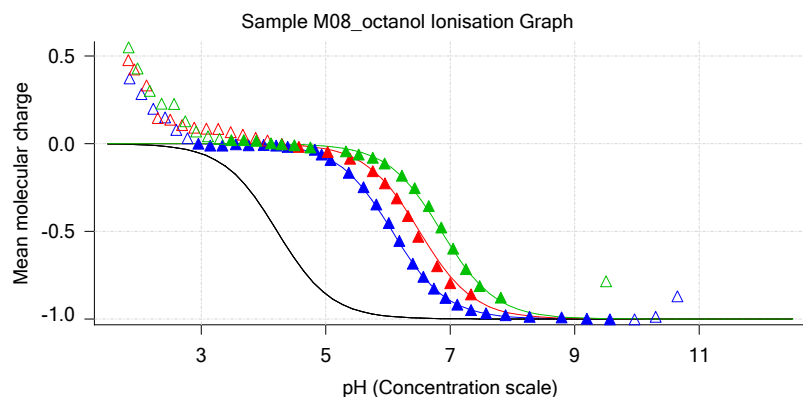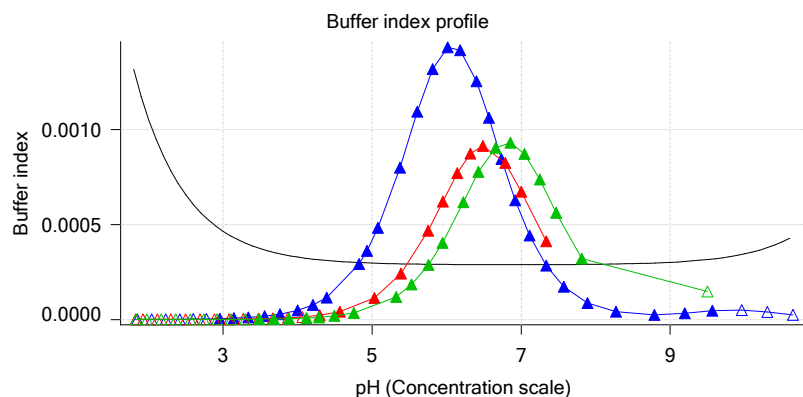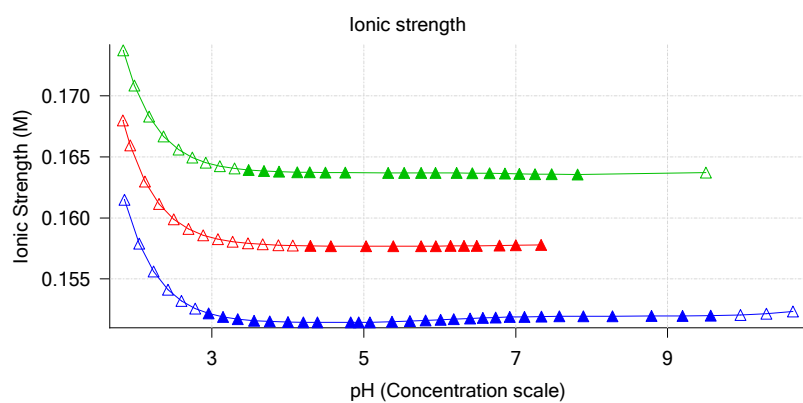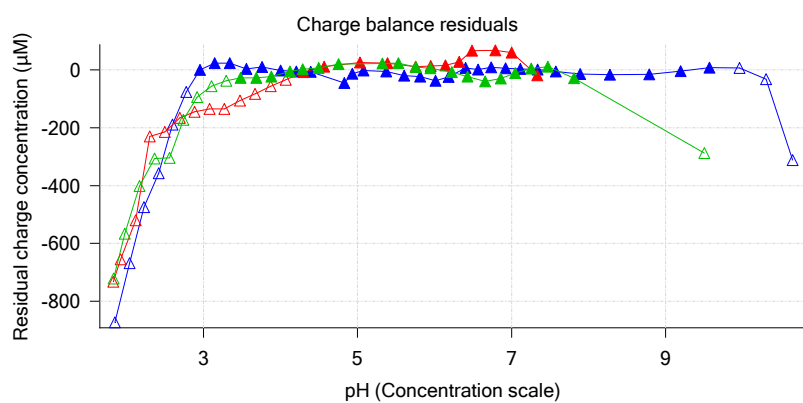
Errors   None
Warnings   None

Sample logD and percent species

pH	M08_octanol logD	M08_octanol M08_octanolH	M08_octanol M08_octanol	M08_octanol M08_octanolH*	M08_octanol M08_octanol*	Comment
1.000	3.16	0.07 %	0.00 %	99.93 %	0.00 %	
1.200	3.16	0.07 %	0.00 %	99.93 %	0.00 %	Stomach pH
2.000	3.16	0.07 %	0.00 %	99.93 %	0.00 %	
3.000	3.13	0.07 %	0.00 %	99.92 %	0.01 %	
4.000	2.95	0.07 %	0.04 %	99.82 %	0.07 %	
5.000	2.32	0.07 %	0.41 %	98.81 %	0.71 %	
6.000	1.40	0.06 %	3.75 %	89.77 %	6.42 %	
6.500	0.97	0.05 %	9.73 %	73.58 %	16.64 %	
7.000	0.61	0.03 %	19.59 %	46.86 %	33.52 %	
7.400	0.43	0.02 %	27.29 %	25.99 %	46.69 %	Blood pH
8.000	0.29	0.01 %	33.90 %	8.11 %	57.99 %	
9.000	0.24	0.00 %	36.57 %	0.87 %	62.56 %	
10.000	0.23	0.00 %	36.86 %	0.09 %	63.05 %	
11.000	0.23	0.00 %	36.89 %	0.01 %	63.10 %	
12.000	0.23	0.00 %	36.89 %	0.00 %	63.11 %	

pH-metric Result

Graphs

Charge balance residuals

Ionic strength

Buffer index profile

Sample M08_octanol Ionisation Graph

Distribution of species for sample M08_octanol

Lipophilicity Profile

Log R Profile

Sample Carbonate Ionisation Graph

Sample name: **M08_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-02009**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02009_M08_octanol_pH-metric high logP.t3r**

Experiment start time: **3/2/2018 8:29:22 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Graphs (continued)

Distribution of species for sample Carbonate

Sample name: **M08_octanol** Experiment start time: **3/2/2018 8:29:22 PM**
Assay name: **pH-metric high logP** Analyst: **Pion**
Assay ID: **18C-02009** Instrument ID: **T312060**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02009_M08_octanol_pH-metric high logP.t3r**

pH-metric high logP   Titration 1 of 3   18C-02009 Points 2 to 38

Overall results

RMSD 0.094
Average ionic strength 0.152 M
Average temperature 25.0°C
Partition ratio 0.0526 : 1
Analyte concentration range 2033.3 µM to 2105.6 µM
Total points considered 28 of 37

Warnings and errors

Errors None
Warnings One or more logP values out of range

Four-Plus parameters

Alpha	0.111	3/2/2018 8:29:22 PM	C:\Sirius_T3\HCl18C02.t3r
S	0.9988	3/2/2018 8:29:22 PM	C:\Sirius_T3\HCl18C02.t3r
jH	1.0	3/2/2018 8:29:22 PM	C:\Sirius_T3\HCl18C02.t3r
jOH	-0.8	3/2/2018 8:29:22 PM	C:\Sirius_T3\HCl18C02.t3r

Titrants

0.50 M HCl	0.999058	3/2/2018 8:29:22 PM	C:\Sirius_T3\HCl18C02.t3r
0.50 M KOH	0.999845	3/2/2018 8:29:22 PM	C:\Sirius_T3\KOH18B27.t3r

Sample

M08_octanol concentration factor 1.095
Acid pKa 1 4.22
logP (neutral XH) 3.13
logP (X -) -5.22

Sample graphs

Ionisation of sample M08_octanol
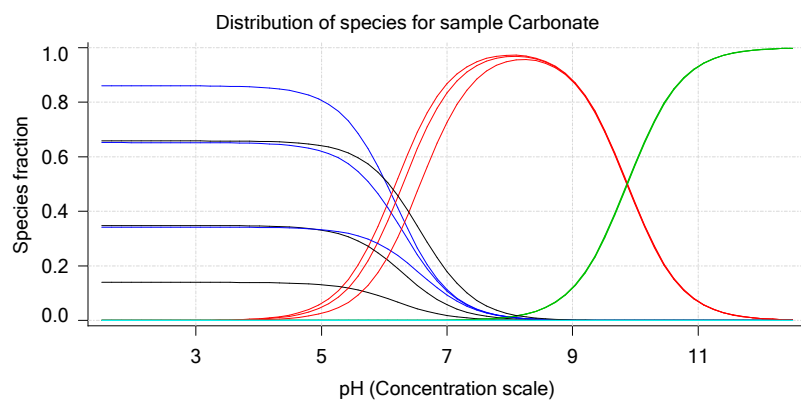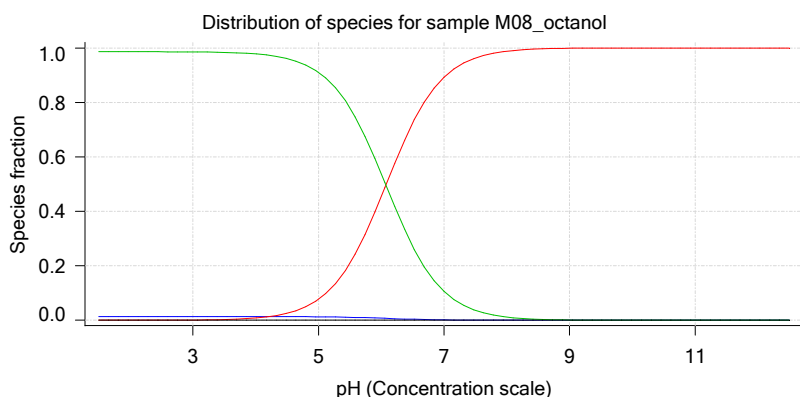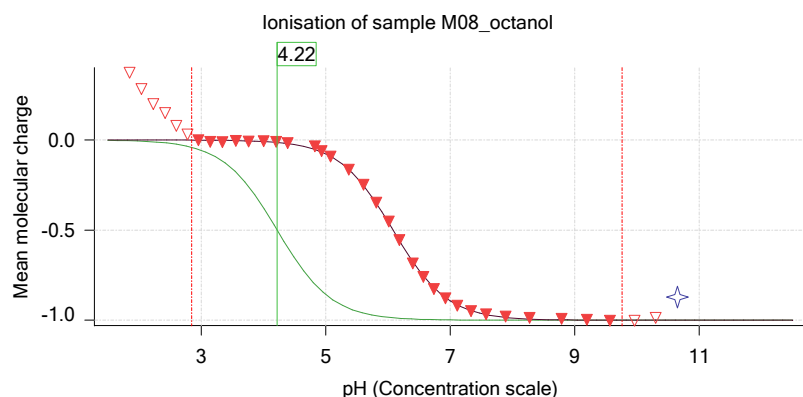

Distribution of species for sample M08_octanol

Sample name: **M08_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-02009**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02009_M08_octanol_pH-metric high logP.t3r**

Experiment start time: **3/2/2018 8:29:22 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Sample graphs (continued)

Lipophilicity Profile
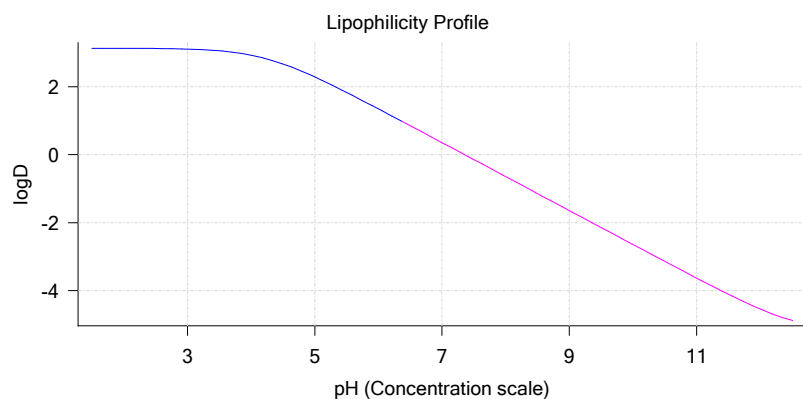
Sample logD and percent species

pH	M08_octanol logD	M08_octanol M08_octanolH	M08_octanol M08_octanol	M08_octanol M08_octanolH*	M08_octanol M08_octanol*	Comment
1.000	3.13	1.38 %	0.00 %	98.62 %	0.00 %	
1.200	3.13	1.38 %	0.00 %	98.62 %	0.00 %	Stomach pH
2.000	3.13	1.38 %	0.01 %	98.61 %	0.00 %	
3.000	3.11	1.38 %	0.08 %	98.54 %	0.00 %	
4.000	2.93	1.37 %	0.82 %	97.81 %	0.00 %	
5.000	2.29	1.27 %	7.67 %	91.06 %	0.00 %	
6.000	1.35	0.75 %	45.38 %	53.86 %	0.00 %	
6.500	0.85	0.38 %	72.43 %	27.19 %	0.00 %	
7.000	0.35	0.15 %	89.26 %	10.59 %	0.00 %	
7.400	-0.05	0.06 %	95.43 %	4.51 %	0.00 %	Blood pH
8.000	-0.65	0.02 %	98.81 %	1.17 %	0.00 %	
9.000	-1.65	0.00 %	99.88 %	0.12 %	0.00 %	
10.000	-2.65	0.00 %	99.99 %	0.01 %	0.00 %	
11.000	-3.64	0.00 %	100.00 %	0.00 %	0.00 %	
12.000	-4.54	0.00 %	100.00 %	0.00 %	0.00 %	

Carbonate and acidity

Carbonate 0.086 mM
Acidity error -0.769 mM

Other graphs
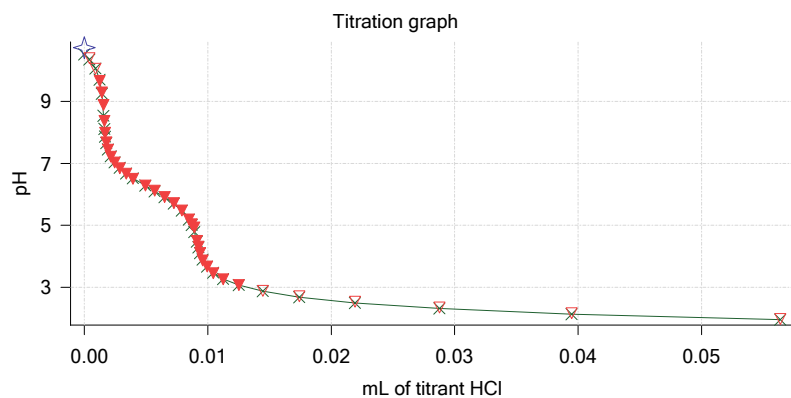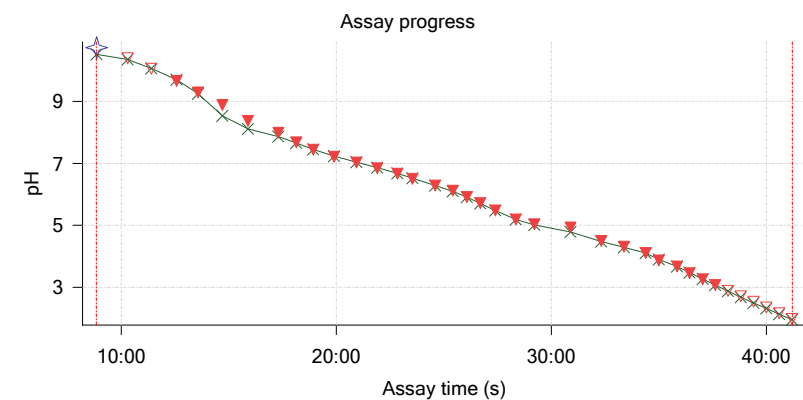
Assay progress

Titration graph

Sample name: **M08_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-02009**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02009_M08_octanol_pH-metric high logP.t3r**

Experiment start time: **3/2/2018 8:29:22 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Other graphs (continued)

Charge balance residuals

Buffer index profile

Ionic strength

Log R Profile

Ionisation of sample Carbonate
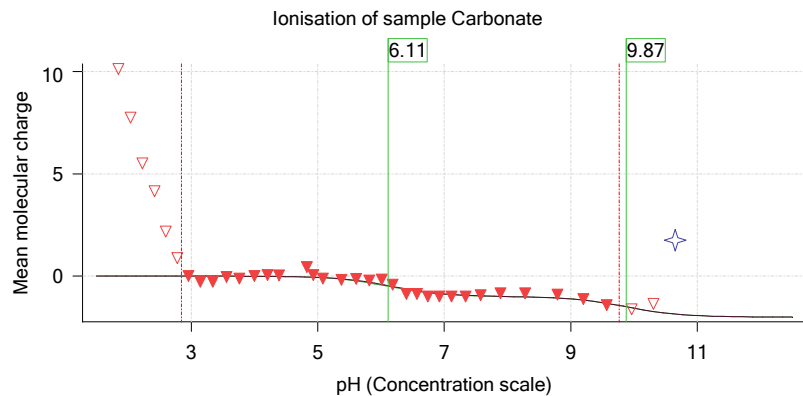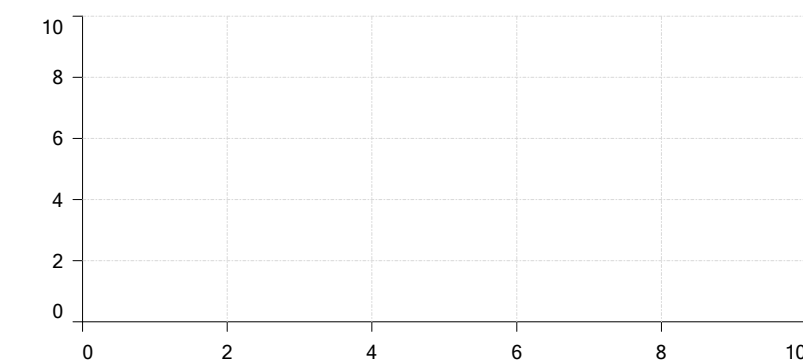
Sample name: **M08_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-02009**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02009_M08_octanol_pH-metric high logP.t3r**

Experiment start time: **3/2/2018 8:29:22 PM**
Analyst: **Pion**
Instrument ID: **T312060**

# pH-metric high logP   Titration 2 of 3   18C-02009 Points 39 to 63

Overall results

RMSD   0.061
Average ionic strength   0.158 M
Average temperature   25.0°C
Partition ratio   0.1728 : 1
Analyte concentration range 1712.1 µM to 1763.3 µM
Total points considered   12 of 25

Warnings and errors

Errors   None
Warnings   One or more logP values out of range

Four-Plus parameters

Alpha   0.111   3/2/2018 8:29:22 PM   C:\Sirius_T3\HCl18C02.t3r
S   0.9988   3/2/2018 8:29:22 PM   C:\Sirius_T3\HCl18C02.t3r
jH   1.0   3/2/2018 8:29:22 PM   C:\Sirius_T3\HCl18C02.t3r
jOH   -0.8   3/2/2018 8:29:22 PM   C:\Sirius_T3\HCl18C02.t3r

Titrants

0.50 M HCl   0.999058   3/2/2018 8:29:22 PM   C:\Sirius_T3\HCl18C02.t3r
0.50 M KOH   0.999845   3/2/2018 8:29:22 PM   C:\Sirius_T3\KOH18B27.t3r

Sample

M08_octanol concentration factor   0.769
Acid pKa 1   4.22
logP (neutral XH)   3.00
logP (X -)   -5.22

Sample graphs

Ionisation of sample M08_octanol

Distribution of species for sample M08_octanol

Sample name: **M08_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-02009**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02009_M08_octanol_pH-metric high logP.t3r**

Experiment start time: **3/2/2018 8:29:22 PM**
Analyst: **Pion**
Instrument ID: **T312060**
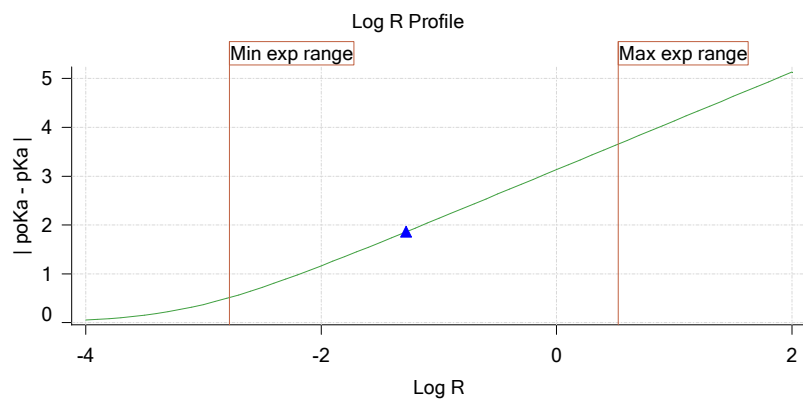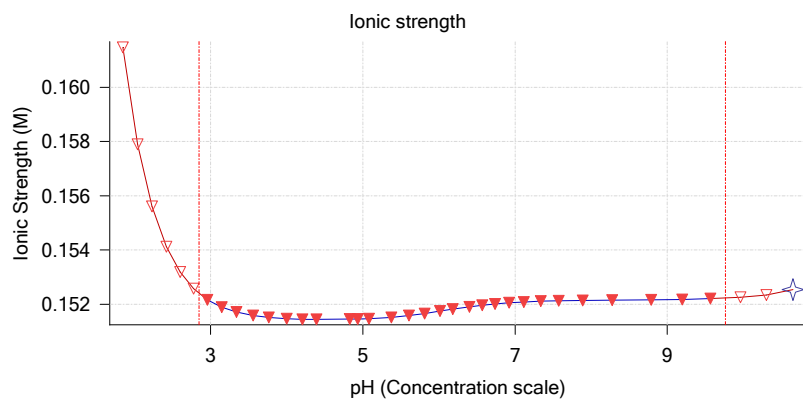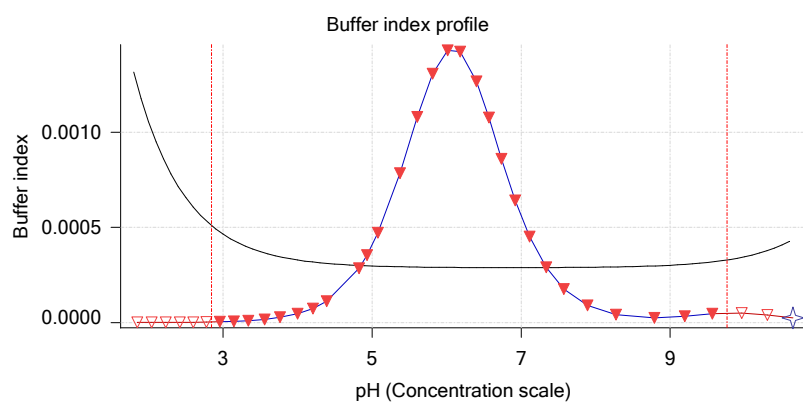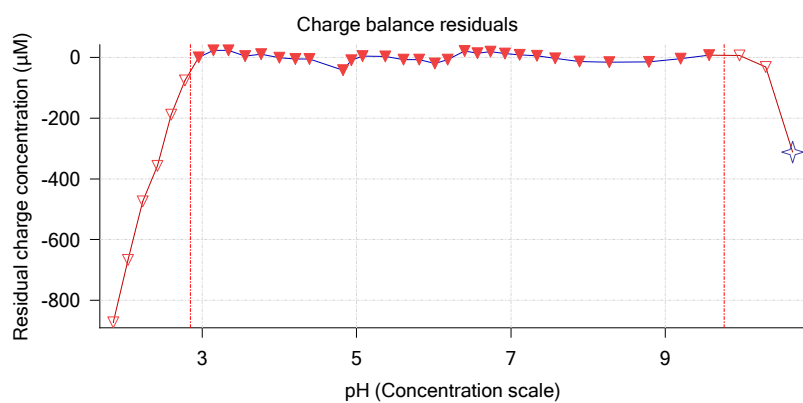
Sample graphs (continued)

Lipophilicity Profile
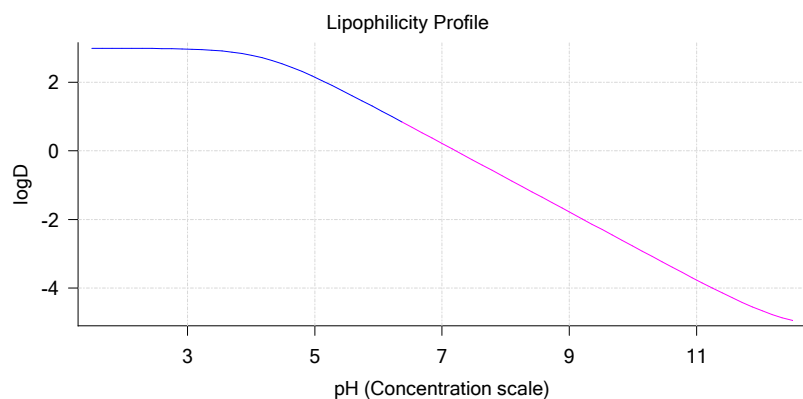
Sample logD and percent species

pH	M08_octanol logD	M08_octanol M08_octanolH	M08_octanol M08_octanol	M08_octanol M08_octanolH*	M08_octanol M08_octanol*	Comment
1.000	3.00	0.58 %	0.00 %	99.42 %	0.00 %	
1.200	3.00	0.58 %	0.00 %	99.42 %	0.00 %	Stomach pH
2.000	2.99	0.58 %	0.00 %	99.42 %	0.00 %	
3.000	2.97	0.58 %	0.03 %	99.39 %	0.00 %	
4.000	2.79	0.58 %	0.35 %	99.07 %	0.00 %	
5.000	2.15	0.56 %	3.38 %	96.06 %	0.00 %	
6.000	1.21	0.43 %	25.90 %	73.67 %	0.00 %	
6.500	0.71	0.28 %	52.50 %	47.23 %	0.00 %	
7.000	0.22	0.13 %	77.75 %	22.12 %	0.00 %	
7.400	-0.18	0.06 %	89.77 %	10.17 %	0.00 %	Blood pH
8.000	-0.78	0.02 %	97.22 %	2.77 %	0.00 %	
9.000	-1.78	0.00 %	99.71 %	0.28 %	0.00 %	
10.000	-2.78	0.00 %	99.97 %	0.03 %	0.00 %	
11.000	-3.77	0.00 %	100.00 %	0.00 %	0.00 %	
12.000	-4.65	0.00 %	100.00 %	0.00 %	0.00 %	

Carbonate and acidity

Carbonate   0.000 mM
Acidity error -0.706 mM

Other graphs
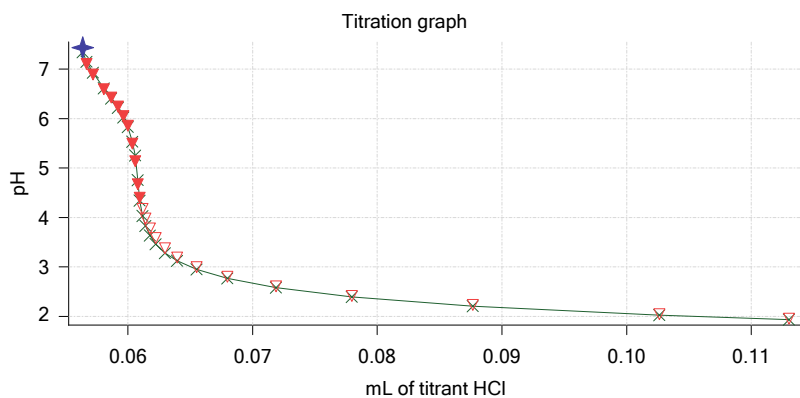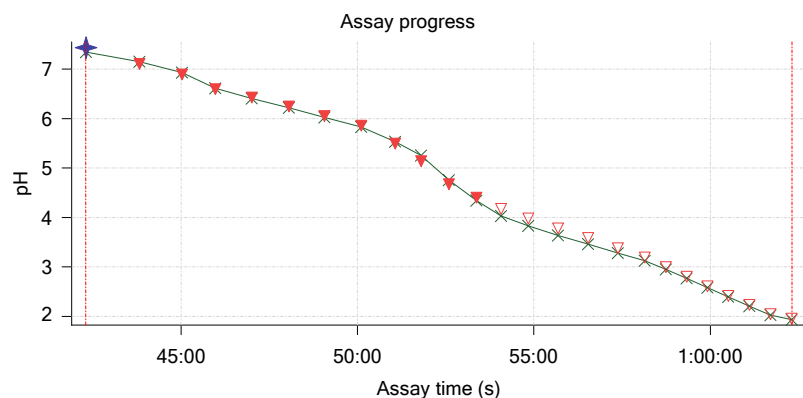
Assay progress

Titration graph

Sample name: **M08_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-02009**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02009_M08_octanol_pH-metric high logP.t3r**

Experiment start time: **3/2/2018 8:29:22 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Other graphs (continued)

Charge balance residuals

Buffer index profile

Ionic strength

Log R Profile

Ionisation of sample Carbonate
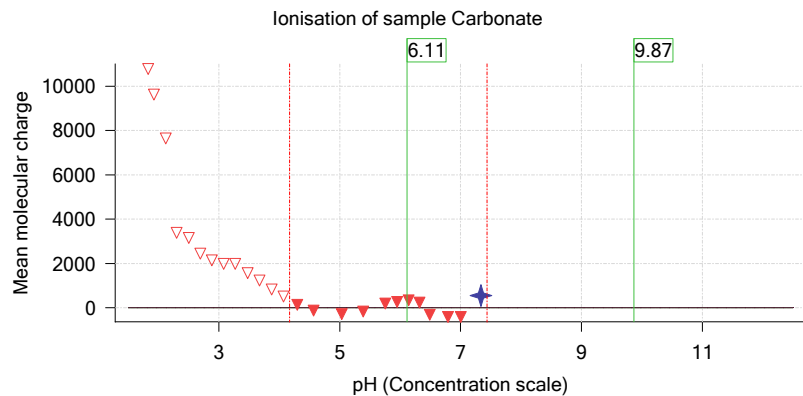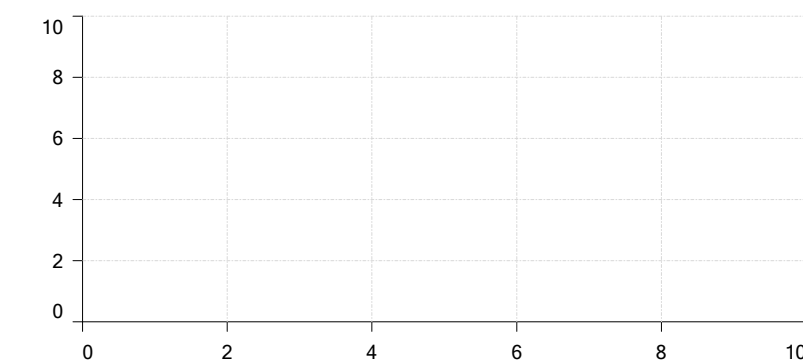
Sample name: **M08_octanol** Experiment start time: **3/2/2018 8:29:22 PM**
Assay name: **pH-metric high logP** Analyst: **Pion**
Assay ID: **18C-02009** Instrument ID: **T312060**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02009_M08_octanol_pH-metric high logP.t3r**

pH-metric high logP   Titration 3 of 3   18C-02009 Points 64 to 92

Overall results

RMSD 0.092
Average ionic strength 0.164 M
Average temperature 25.0°C
Partition ratio 0.6226 : 1
Analyte concentration range 1164.0 µM to 1189.2 µM
Total points considered 19 of 29

Warnings and errors

Errors None
Warnings One or more logP values out of range

Four-Plus parameters

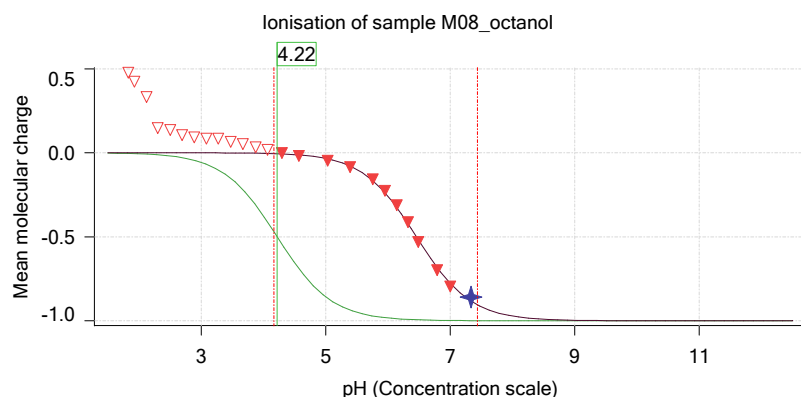|			
Alpha	0.111	3/2/2018 8:29:22 PM	C:\Sirius_T3\HCl18C02.t3r
S	0.9988	3/2/2018 8:29:22 PM	C:\Sirius_T3\HCl18C02.t3r
jH	1.0	3/2/2018 8:29:22 PM	C:\Sirius_T3\HCl18C02.t3r
jOH	-0.8	3/2/2018 8:29:22 PM	C:\Sirius_T3\HCl18C02.t3r

Titrants

0.50 M HCl	0.999058	3/2/2018 8:29:22 PM	C:\Sirius_T3\HCl18C02.t3r
0.50 M KOH	0.999845	3/2/2018 8:29:22 PM	C:\Sirius_T3\KOH18B27.t3r

Sample

M08_octanol concentration factor 0.703
Acid pKa 1 4.22
logP (neutral XH) 2.87
logP (X -) -5.22

Sample graphs

Ionisation of sample M08_octanol

Distribution of species for sample M08_octanol

Sample name: **M08_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-02009**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02009_M08_octanol_pH-metric high logP.t3r**

Experiment start time: **3/2/2018 8:29:22 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Sample graphs (continued)

Lipophilicity Profile
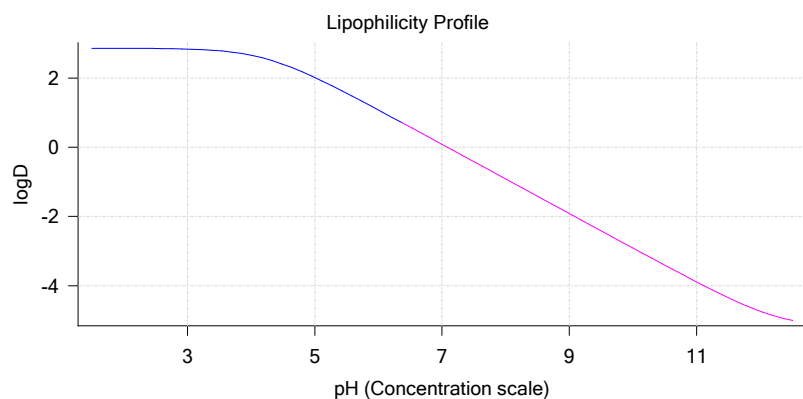
Sample logD and percent species

pH	M08_octanol logD	M08_octanol M08_octanolH	M08_octanol M08_octanol	M08_octanol M08_octanolH*	M08_octanol M08_octanol*	Comment
1.000	2.86	0.22 %	0.00 %	99.78 %	0.00 %	
1.200	2.86	0.22 %	0.00 %	99.78 %	0.00 %	Stomach pH
2.000	2.86	0.22 %	0.00 %	99.78 %	0.00 %	
3.000	2.84	0.22 %	0.01 %	99.77 %	0.00 %	
4.000	2.66	0.22 %	0.13 %	99.65 %	0.00 %	
5.000	2.02	0.22 %	1.30 %	98.48 %	0.00 %	
6.000	1.08	0.19 %	11.64 %	88.17 %	0.00 %	
6.500	0.58	0.15 %	29.40 %	70.44 %	0.00 %	
7.000	0.08	0.09 %	56.84 %	43.06 %	0.00 %	
7.400	-0.32	0.05 %	76.79 %	23.16 %	0.00 %	Blood pH
8.000	-0.91	0.02 %	92.94 %	7.04 %	0.00 %	
9.000	-1.91	0.00 %	99.25 %	0.75 %	0.00 %	
10.000	-2.91	0.00 %	99.92 %	0.08 %	0.00 %	
11.000	-3.89	0.00 %	99.99 %	0.01 %	0.00 %	
12.000	-4.74	0.00 %	100.00 %	0.00 %	0.00 %	

Carbonate and acidity

Carbonate   0.288 mM
Acidity error   -0.437 mM

Other graphs

Assay progress

Titration graph
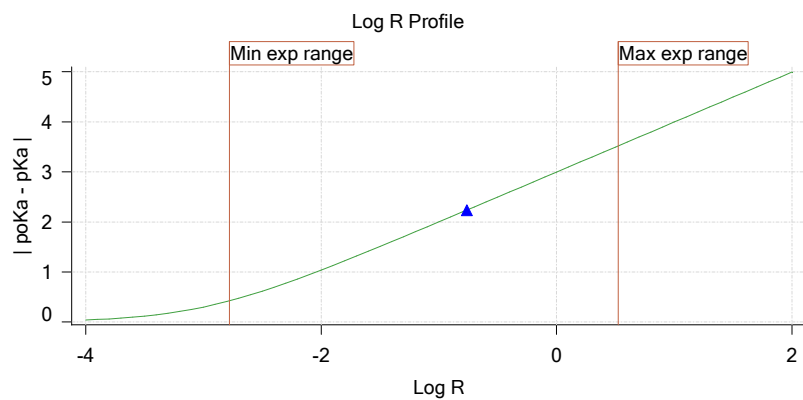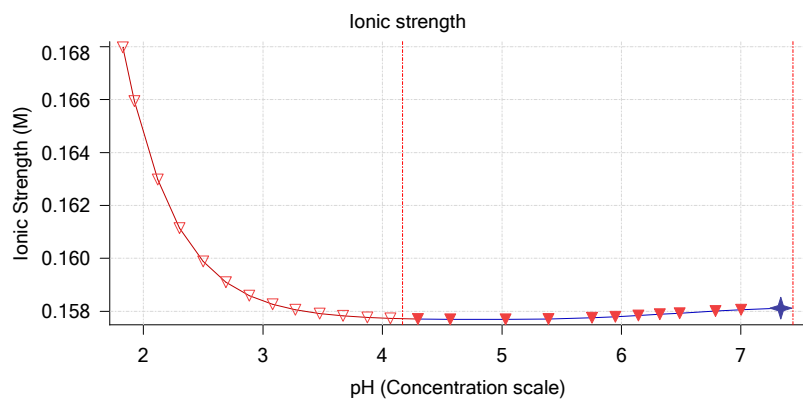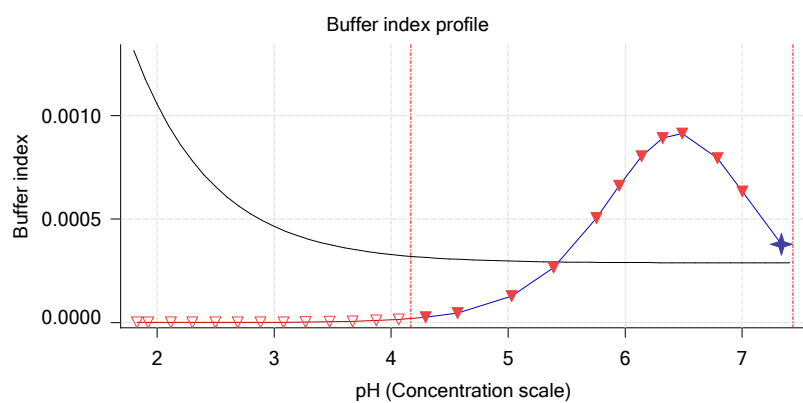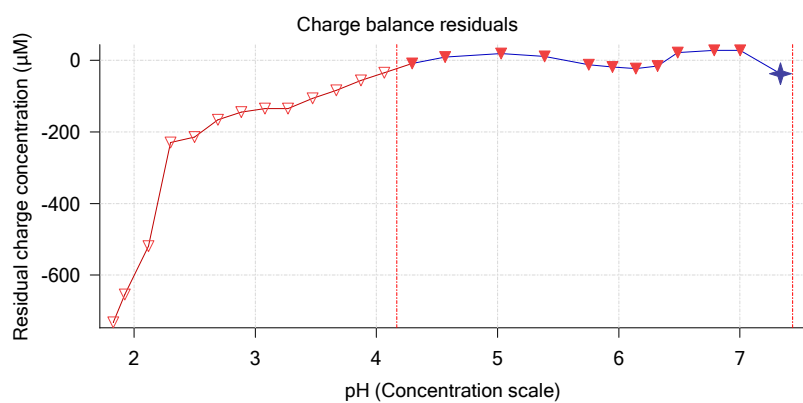
Sample name: **M08_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-02009**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02009_M08_octanol_pH-metric high logP.t3r**

Experiment start time: **3/2/2018 8:29:22 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Other graphs (continued)

Charge balance residuals

Buffer index profile

Ionic strength

Log R Profile

Ionisation of sample Carbonate
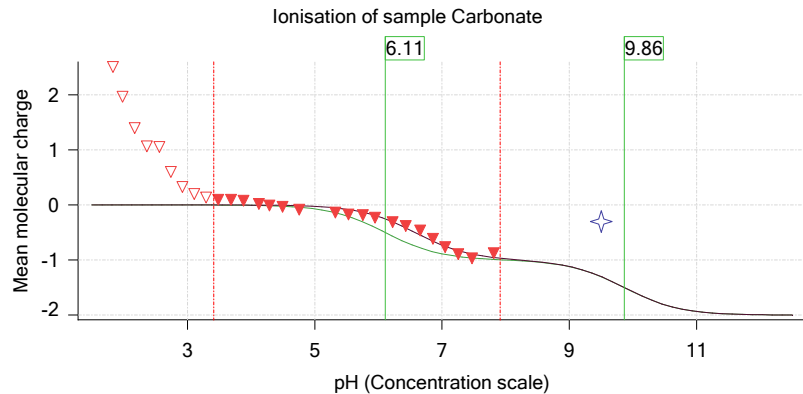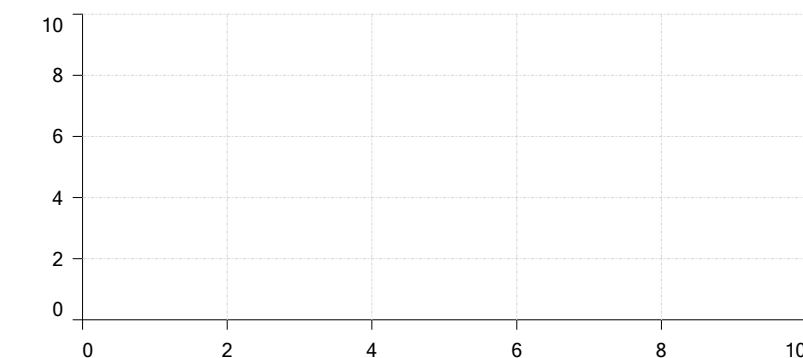
Assay model

Sample name: **M08_octanol**

Assay name: **pH-metric high logP**

Assay ID: **18C-02009**

Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02009_M08_octanol_pH-metric high logP.t3r**

Experiment start time: **3/2/2018 8:29:22 PM**

Analyst: **Pion**

Instrument ID: **T312060**

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	M08_octanol	2/27/2018 4:33:51 PM	User entered value
Sample by	Weight		Default value
Sample weight	0.000980 g	3/2/2018 5:08:22 PM	User entered value
Formula weight	293.32 g/mol	2/27/2018 4:33:51 PM	User entered value
Solubility	Unknown		Default value
Molecular weight	293.32	2/27/2018 4:33:51 PM	User entered value
Individual pKa ionic environments	No		Default value
Number of pKas	1	2/27/2018 4:33:51 PM	User entered value
Sample is a	Acid	2/27/2018 4:33:51 PM	User entered value
pKa 1	4.22	2/27/2018 4:33:51 PM	User entered value
logP (neutral XH)	2.98	3/2/2018 3:22:58 PM	User entered value
logP (X -)	-5.22	3/2/2018 3:23:03 PM	User entered value

Events

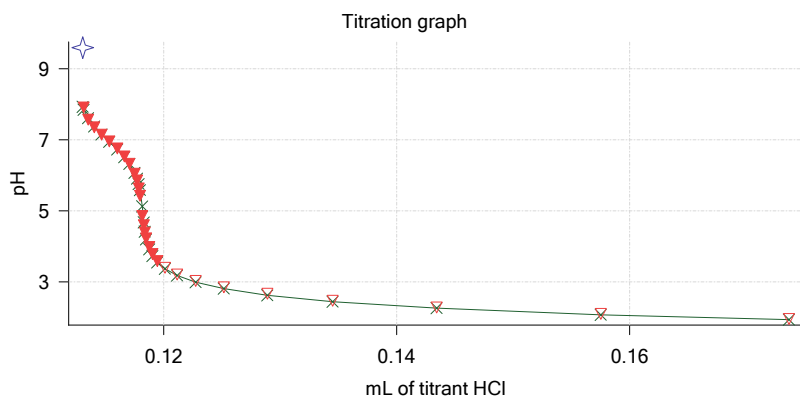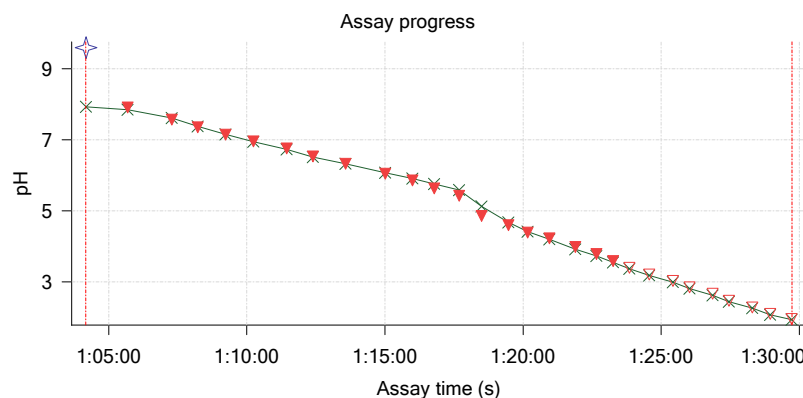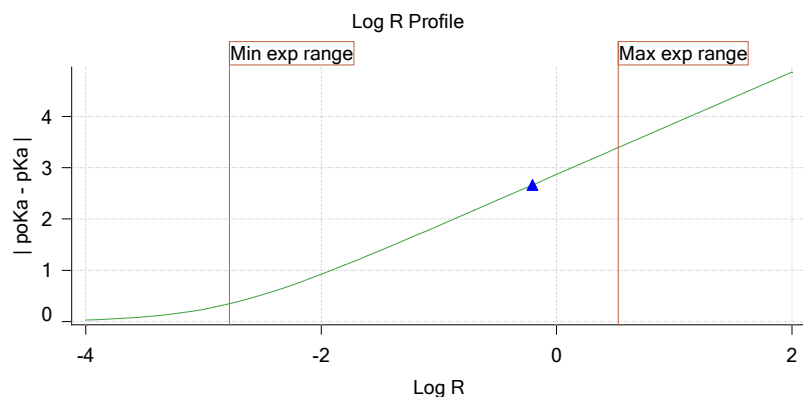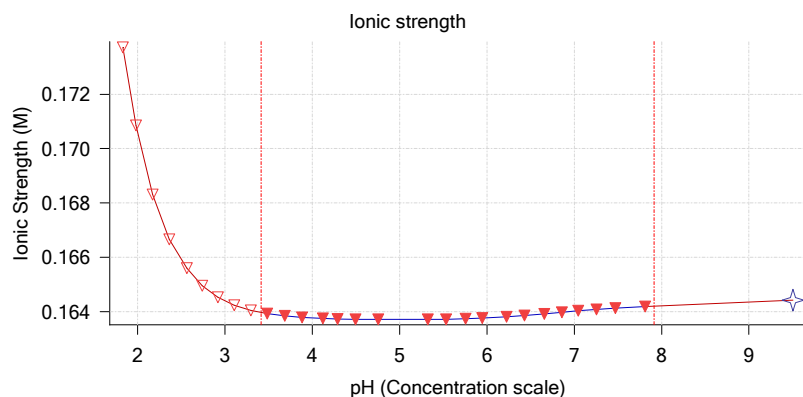| Time	Event	Water	Acid	Base	Octanol	pH	dpH/dt	pH R-squared	pH SD	dpH time
5:58.3	Manual volume addition				0.08000 mL					
5:59.4	Initial pH = 5.13									
8:51.4	Data point 2	1.50000 mL	0.00000 mL	0.00680 mL	0.08000 mL	10.746	-0.11246	0.99456	0.00557	Timed out at
10:18.0	Data point 3	1.50000 mL	0.00042 mL	0.00680 mL	0.08000 mL	10.400	0.01868	0.91894	0.00096	35.0 s
11:23.6	Data point 4	1.50000 mL	0.00092 mL	0.00680 mL	0.08000 mL	10.058	0.01821	0.90743	0.00094	40.5 s
12:34.8	Data point 5	1.50000 mL	0.00125 mL	0.00680 mL	0.08000 mL	9.666	-0.01373	0.55829	0.00091	28.5 s
13:33.8	Data point 6	1.50000 mL	0.00143 mL	0.00680 mL	0.08000 mL	9.296	-0.01475	0.60041	0.00094	32.5 s
14:42.1	Data point 7	1.50000 mL	0.00155 mL	0.00680 mL	0.08000 mL	8.888	-0.01820	0.87464	0.00096	36.0 s
15:53.7	Data point 8	1.50000 mL	0.00162 mL	0.00680 mL	0.08000 mL	8.376	-0.01780	0.85957	0.00095	49.0 s
17:18.5	Data point 9	1.50000 mL	0.00169 mL	0.00680 mL	0.08000 mL	7.991	0.00108	0.00290	0.00099	19.5 s
18:08.5	Data point 10	1.50000 mL	0.00179 mL	0.00680 mL	0.08000 mL	7.676	0.01522	0.69377	0.00090	17.0 s
18:56.0	Data point 11	1.50000 mL	0.00193 mL	0.00680 mL	0.08000 mL	7.439	0.01692	0.86099	0.00090	17.0 s
19:53.8	Data point 12	1.50000 mL	0.00216 mL	0.00680 mL	0.08000 mL	7.216	0.01704	0.82585	0.00093	21.0 s
20:55.8	Data point 13	1.50000 mL	0.00247 mL	0.00680 mL	0.08000 mL	7.024	0.01724	0.88730	0.00090	17.0 s
21:53.7	Data point 14	1.50000 mL	0.00287 mL	0.00680 mL	0.08000 mL	6.840	0.01697	0.84626	0.00091	16.0 s
22:50.5	Data point 15	1.50000 mL	0.00339 mL	0.00680 mL	0.08000 mL	6.669	0.01841	0.84076	0.00099	16.5 s
23:32.5	Data point 16	1.50000 mL	0.00395 mL	0.00680 mL	0.08000 mL	6.504	0.01741	0.89494	0.00091	17.0 s
24:35.6	Data point 17	1.50000 mL	0.00494 mL	0.00680 mL	0.08000 mL	6.285	0.01783	0.92060	0.00092	13.5 s
25:24.8	Data point 18	1.50000 mL	0.00571 mL	0.00680 mL	0.08000 mL	6.116	0.01844	0.92964	0.00095	13.5 s
26:03.8	Data point 19	1.50000 mL	0.00651 mL	0.00680 mL	0.08000 mL	5.916	0.01893	0.91741	0.00098	12.5 s
26:41.7	Data point 20	1.50000 mL	0.00727 mL	0.00680 mL	0.08000 mL	5.710	0.01949	0.97281	0.00098	16.0 s

Sample name: **M08_octanol** Experiment start time: **3/2/2018 8:29:22 PM**
Assay name: **pH-metric high logP** Analyst: **Pion**
Assay ID: **18C-02009** Instrument ID: **T312060**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02009_M08_octanol_pH-metric high logP.t3r**

Events (continued)

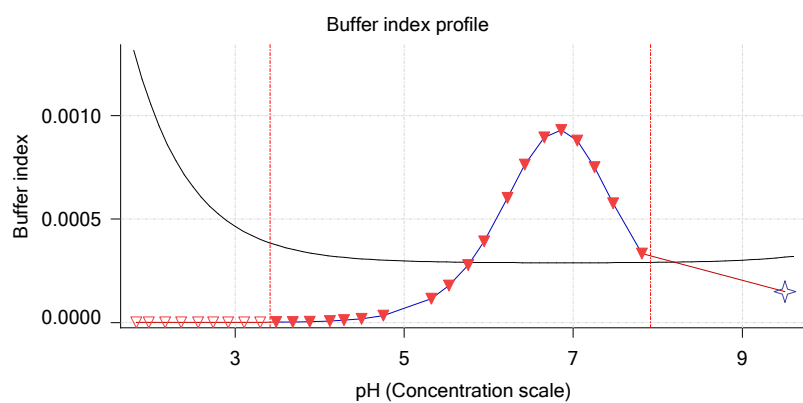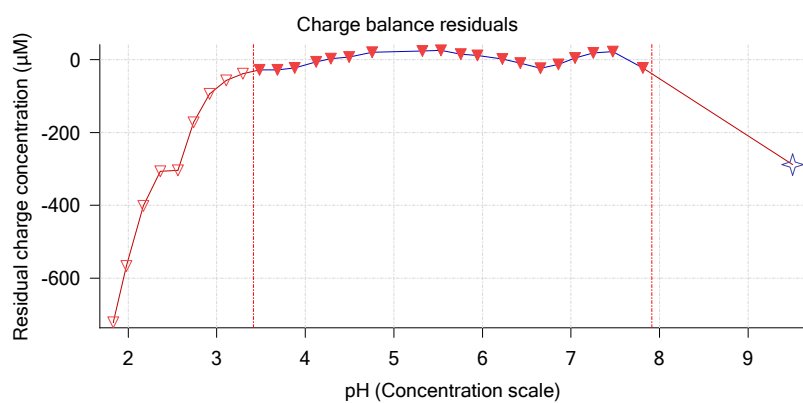| Time	Event	Water	Acid	Base	Octanol	pH	dpH/dt	pH R-squared	pH SD	dpH/dt time
27:23.2	Data point 21	1.50000 mL	0.00790 mL	0.00680 mL	0.08000 mL	5.477	0.01911	0.96079	0.00096	17.0 s
28:21.0	Data point 22	1.50000 mL	0.00847 mL	0.00680 mL	0.08000 mL	5.183	0.01836	0.88513	0.00096	21.0 s
29:12.6	Data point 23	1.50000 mL	0.00870 mL	0.00680 mL	0.08000 mL	5.036	0.05948	0.99622	0.00294	Timed out at 59.5 s
30:53.3	Data point 24	1.50000 mL	0.00891 mL	0.00680 mL	0.08000 mL	4.931	0.05785	0.99230	0.00287	Timed out at 59.5 s
32:18.7	Data point 25	1.50000 mL	0.00913 mL	0.00680 mL	0.08000 mL	4.496	0.01948	0.93912	0.00099	33.0 s
33:22.3	Data point 26	1.50000 mL	0.00924 mL	0.00680 mL	0.08000 mL	4.310	0.01919	0.92386	0.00099	25.5 s
34:23.5	Data point 27	1.50000 mL	0.00938 mL	0.00680 mL	0.08000 mL	4.106	0.01620	0.92889	0.00083	10.5 s
34:59.4	Data point 28	1.50000 mL	0.00960 mL	0.00680 mL	0.08000 mL	3.868	0.01215	0.93122	0.00062	10.0 s
35:50.2	Data point 29	1.50000 mL	0.00995 mL	0.00680 mL	0.08000 mL	3.663	0.01206	0.86827	0.00064	10.0 s
36:25.7	Data point 30	1.50000 mL	0.01044 mL	0.00680 mL	0.08000 mL	3.447	0.00079	0.06082	0.00016	10.5 s
37:01.6	Data point 31	1.50000 mL	0.01124 mL	0.00680 mL	0.08000 mL	3.252	0.00291	0.66841	0.00018	10.0 s
37:37.1	Data point 32	1.50000 mL	0.01251 mL	0.00680 mL	0.08000 mL	3.063	0.00379	0.17037	0.00045	10.0 s
38:12.6	Data point 33	1.50000 mL	0.01446 mL	0.00680 mL	0.08000 mL	2.886	-0.00068	0.10900	0.00010	10.0 s
38:48.2	Data point 34	1.50000 mL	0.01743 mL	0.00680 mL	0.08000 mL	2.708	-0.00988	0.27293	0.00093	10.0 s
39:23.8	Data point 35	1.50000 mL	0.02192 mL	0.00680 mL	0.08000 mL	2.530	-0.00487	0.81957	0.00027	10.0 s
39:59.3	Data point 36	1.50000 mL	0.02876 mL	0.00680 mL	0.08000 mL	2.343	-0.01064	0.51106	0.00073	10.0 s
40:35.0	Data point 37	1.50000 mL	0.03949 mL	0.00680 mL	0.08000 mL	2.157	-0.01066	0.81291	0.00058	10.0 s
41:10.9	Data point 38	1.50000 mL	0.05637 mL	0.00680 mL	0.08000 mL	1.971	-0.01287	0.96844	0.00065	10.5 s
42:18.9	Data point 39	1.50000 mL	0.05637 mL	0.05847 mL	0.28000 mL	7.437	-0.14549	0.99322	0.00721	Timed out at 59.5 s
43:49.4	Data point 40	1.50000 mL	0.05670 mL	0.05847 mL	0.28000 mL	7.103	-0.01286	0.42347	0.00098	36.5 s
45:01.7	Data point 41	1.50000 mL	0.05720 mL	0.05847 mL	0.28000 mL	6.891	0.01894	0.94814	0.00096	21.0 s
45:58.4	Data point 42	1.50000 mL	0.05807 mL	0.05847 mL	0.28000 mL	6.590	0.01908	0.89638	0.00100	26.5 s
47:00.7	Data point 43	1.50000 mL	0.05868 mL	0.05847 mL	0.28000 mL	6.423	0.01918	0.91840	0.00099	27.0 s
48:03.4	Data point 44	1.50000 mL	0.05920 mL	0.05847 mL	0.28000 mL	6.245	0.01858	0.85197	0.00099	25.0 s
49:04.1	Data point 45	1.50000 mL	0.05964 mL	0.05847 mL	0.28000 mL	6.052	0.01835	0.93095	0.00094	26.5 s
50:06.3	Data point 46	1.50000 mL	0.06000 mL	0.05847 mL	0.28000 mL	5.858	0.01996	0.97913	0.00100	22.0 s
51:04.1	Data point 47	1.50000 mL	0.06037 mL	0.05847 mL	0.28000 mL	5.493	0.01776	0.89690	0.00093	19.0 s
51:48.5	Data point 48	1.50000 mL	0.06058 mL	0.05847 mL	0.28000 mL	5.135	0.01954	0.96361	0.00098	16.5 s
52:35.6	Data point 49	1.50000 mL	0.06079 mL	0.05847 mL	0.28000 mL	4.673	0.01944	0.94099	0.00099	16.0 s
53:22.2	Data point 50	1.50000 mL	0.06096 mL	0.05847 mL	0.28000 mL	4.401	0.01686	0.77173	0.00095	11.5 s
54:04.2	Data point 51	1.50000 mL	0.06117 mL	0.05847 mL	0.28000 mL	4.172	0.01841	0.83644	0.00099	10.5 s
54:50.4	Data point 52	1.50000 mL	0.06141 mL	0.05847 mL	0.28000 mL	3.979	0.00270	0.11201	0.00040	10.0 s
55:41.2	Data point 53	1.50000 mL	0.06176 mL	0.05847 mL	0.28000 mL	3.777	0.00199	0.23344	0.00020	10.0 s
56:32.1	Data point 54	1.50000 mL	0.06223 mL	0.05847 mL	0.28000 mL	3.582	0.00442	0.54450	0.00030	10.0 s
57:23.0	Data point 55	1.50000 mL	0.06298 mL	0.05847 mL	0.28000 mL	3.377	-0.00183	0.13137	0.00025	10.0 s
58:08.8	Data point 56	1.50000 mL	0.06395 mL	0.05847 mL	0.28000 mL	3.187	-0.00575	0.75760	0.00033	10.0 s
58:44.2	Data point 57	1.50000 mL	0.06552 mL	0.05847 mL	0.28000 mL	2.993	-0.00768	0.67458	0.00046	10.0 s
59:19.7	Data point 58	1.50000 mL	0.06799 mL	0.05847 mL	0.28000 mL	2.800	-0.00920	0.23870	0.00093	10.0 s
59:55.3	Data point 59	1.50000 mL	0.07187 mL	0.05847 mL	0.28000 mL	2.609	-0.00893	0.93688	0.00046	10.0 s
1:00:30.9	Data point 60	1.50000 mL	0.07796 mL	0.05847 mL	0.28000 mL	2.414	-0.01402	0.81271	0.00077	10.0 s
1:01:06.6	Data point 61	1.50000 mL	0.08765 mL	0.05847 mL	0.28000 mL	2.234	-0.01252	0.94599	0.00064	10.0 s
1:01:42.4	Data point 62	1.50000 mL	0.10263 mL	0.05847 mL	0.28000 mL	2.045	-0.01296	0.81107	0.00071	10.0 s
1:02:18.1	Data point 63	1.50000 mL	0.11303 mL	0.05847 mL	0.28000 mL	1.952	-0.01017	0.74429	0.00058	10.0 s
1:04:11.0	Data point 64	1.50000 mL	0.11303 mL	0.11660 mL	1.08000 mL	9.602	-0.07572	0.97633	0.00379	Timed out at 59.5 s
1:05:41.5	Data point 65	1.50000 mL	0.11312 mL	0.11660 mL	1.08000 mL	7.914	-0.01009	0.17302	0.00120	Timed out at 59.5 s
1:07:17.2	Data point 66	1.50000 mL	0.11350 mL	0.11660 mL	1.08000 mL	7.574	0.00521	0.07080	0.00097	20.5 s
1:08:13.4	Data point 67	1.50000 mL	0.11402 mL	0.11660 mL	1.08000 mL	7.354	0.00770	0.15435	0.00097	25.0 s
1:09:14.2	Data point 68	1.50000 mL	0.11465 mL	0.11660 mL	1.08000 mL	7.149	0.01456	0.60986	0.00092	24.5 s
1:10:14.4	Data point 69	1.50000 mL	0.11531 mL	0.11660 mL	1.08000 mL	6.960	0.01422	0.79037	0.00079	31.5 s
1:11:26.9	Data point 70	1.50000 mL	0.11599 mL	0.11660 mL	1.08000 mL	6.759	0.01621	0.64775	0.00100	31.5 s
1:12:23.9	Data point 71	1.50000 mL	0.11660 mL	0.11660 mL	1.08000 mL	6.531	0.01843	0.87072	0.00098	45.0 s
1:13:34.3	Data point 72	1.50000 mL	0.11705 mL	0.11660 mL	1.08000 mL	6.327	0.01609	0.74484	0.00092	40.5 s

Sample name: **M08_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-02009**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02009_M08_octanol_pH-metric high logP.t3r**

Experiment start time: **3/2/2018 8:29:22 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Events (continued)

Time	Event	Water	Acid	Base	Octanol	pH	dpH/dt	pH R-squared	pH SD	dpH/dt time
1:15:00.9	Data point 73	1.50000 mL	0.11750 mL	0.11660 mL	1.08000 mL	6.048	0.00782	0.18941	0.00089	23.5 s
1:16:00.0	Data point 74	1.50000 mL	0.11771 mL	0.11660 mL	1.08000 mL	5.859	0.00920	0.23435	0.00094	21.5 s
1:16:46.9	Data point 75	1.50000 mL	0.11785 mL	0.11660 mL	1.08000 mL	5.634	0.01897	0.91284	0.00098	24.0 s
1:17:41.5	Data point 76	1.50000 mL	0.11797 mL	0.11660 mL	1.08000 mL	5.426	0.01127	0.33431	0.00097	18.0 s
1:18:30.1	Data point 77	1.50000 mL	0.11816 mL	0.11660 mL	1.08000 mL	4.860	0.01580	0.66582	0.00096	22.5 s
1:19:28.2	Data point 78	1.50000 mL	0.11827 mL	0.11660 mL	1.08000 mL	4.601	-0.00526	0.07244	0.00097	11.5 s
1:20:10.2	Data point 79	1.50000 mL	0.11837 mL	0.11660 mL	1.08000 mL	4.394	0.01090	0.29750	0.00099	21.5 s
1:20:57.2	Data point 80	1.50000 mL	0.11848 mL	0.11660 mL	1.08000 mL	4.228	0.00338	0.03554	0.00089	10.5 s
1:21:53.7	Data point 81	1.50000 mL	0.11874 mL	0.11660 mL	1.08000 mL	3.988	-0.01055	0.71176	0.00062	10.0 s
1:22:39.4	Data point 82	1.50000 mL	0.11903 mL	0.11660 mL	1.08000 mL	3.791	-0.01849	0.93115	0.00095	10.5 s
1:23:15.3	Data point 83	1.50000 mL	0.11945 mL	0.11660 mL	1.08000 mL	3.591	-0.01497	0.62245	0.00094	10.0 s
1:23:50.8	Data point 84	1.50000 mL	0.12011 mL	0.11660 mL	1.08000 mL	3.403	0.01050	0.27436	0.00099	18.0 s
1:24:34.2	Data point 85	1.50000 mL	0.12114 mL	0.11660 mL	1.08000 mL	3.213	0.00072	0.00159	0.00089	25.5 s
1:25:25.3	Data point 86	1.50000 mL	0.12274 mL	0.11660 mL	1.08000 mL	3.027	-0.00532	0.13136	0.00073	10.5 s
1:26:01.3	Data point 87	1.50000 mL	0.12517 mL	0.11660 mL	1.08000 mL	2.849	-0.00610	0.09602	0.00097	25.0 s
1:26:51.9	Data point 88	1.50000 mL	0.12888 mL	0.11660 mL	1.08000 mL	2.672	-0.01765	0.96186	0.00089	10.0 s
1:27:27.4	Data point 89	1.50000 mL	0.13450 mL	0.11660 mL	1.08000 mL	2.475	-0.00467	0.05593	0.00097	24.5 s
1:28:17.7	Data point 90	1.50000 mL	0.14344 mL	0.11660 mL	1.08000 mL	2.286	-0.01613	0.73740	0.00093	13.5 s
1:28:56.9	Data point 91	1.50000 mL	0.15753 mL	0.11660 mL	1.08000 mL	2.098	0.00368	0.03491	0.00097	20.5 s
1:29:43.3	Data point 92	1.50000 mL	0.17368 mL	0.11660 mL	1.08000 mL	1.955	0.00356	0.03439	0.00095	19.5 s
1:30:11.8	Assay volumes	1.50000 mL	0.17368 mL	0.11660 mL	1.08000 mL					

Sample name: **M08_octanol**　　　　　　　　　Experiment start time: **3/2/2018 8:29:22 PM**
Assay name: **pH-metric high logP**　　　　　　Analyst: **Pion**
Assay ID: **18C-02009**　　　　　　　　　　　Instrument ID: **T312060**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02009_M08_octanol_pH-metric high logP.t3r**

Assay Settings

Setting	Value	Original Value	Date/Time changed	Imported from
General Settings				
Analyst name	Pion			
Standard Experiment Settings				
Number of titrations	3			
Minimum pH	2.000			
Maximum pH	10.000			
pH step between points of	0.200			
Minimum titrant addition	0.00002 mL			
Maximum titrant addition	0.10000 mL			
Argon flow rate	100%			
Start titration using	Cautious pH adjust			
Advanced General Settings				
Detect turbidity using	None			
Collect turbidity sensor data	No			
Collect UV spectra	No			
Stir after titrant addition for	5 seconds			
For titrant addition, stir at	10%			
Titrant Pre-Dose				
Titrant pre-dose	None			
Assay Medium				
ISA water volume	1.50 mL			
Water added	Automatic			
Partition solvent type	Octanol			
Partition volume	0.080 mL			
Partition solvent added	Manual in advance			
After partition addition, stir for	1 seconds			
Sample Sonication				
Sonicate	Yes			
Adjust pH for sonication	No			
Sonicate for	120 seconds			
After sonication stir for	5 seconds			
Sample Dissolution				
Perform a dissolution stage	Yes			
Adjust and hold pH for dissolution	To start pH			
Stir to dissolve for	120 seconds			
For dissolution, stir at	10%			
Carbonate purge				
Perform a carbonate purge	No			
Temperature Control				
Wait for temperature	Yes			
Required start temperature	25.0°C			
Acceptable deviation	0.5°C			
Time to wait	60 seconds			
Stir speed of	50%			
Titration 1				
Titrate from	High to low pH			
Adjust to start pH	Yes			
After pH adjust stir for	30 seconds			
Stir to allow partitioning for	15 seconds			
Stirrer speed for partitioning	50%			
Titration 2				
Titrate from	High to low pH			
Add additional water	0.00 mL			
Additional partition solvent volume	0.200 mL			
Additional partition solvent added	Automatic			
After pH adjust stir for	30 seconds			
Stir to allow partitioning for	15 seconds			
Stirrer speed for partitioning	55%			

Sample name: **M08_octanol**
Assay name: **pH-metric high logP**
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Experiment start time: **3/2/2018 8:29:22 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Assay Settings (continued)

Setting	Value	Original Value	Date/Time changed	Imported from
Titration 3				
Titrate from	High to low pH			
Add additional water	0.00 mL			
Additional partition solvent volume	0.800 mL			
Additional partition solvent added	Automatic			
After pH adjust stir for	30 seconds			
Stir to allow partitioning for	15 seconds			
Stirrer speed for partitioning	60%			
Data Point Stability				
Stir during data point collection	No			
Delay before data point collection	0 seconds			
Number of points to average	20 points			
Time interval between points	0.50 seconds			
Required maximum standard deviation	0.00100 dpH/dt			
Stability timeout after	60 seconds			

Calibration Settings

Setting	Value	Date/Time changed	Imported from
Four-Plus alpha	0.111	3/2/2018 8:29:22 PM	C:\Sirius_T3\HCl18C02.t3r
Four-Plus S	0.9988	3/2/2018 8:29:22 PM	C:\Sirius_T3\HCl18C02.t3r
Four-Plus jH	1.0	3/2/2018 8:29:22 PM	C:\Sirius_T3\HCl18C02.t3r
Four-Plus jOH	-0.8	3/2/2018 8:29:22 PM	C:\Sirius_T3\HCl18C02.t3r
Base concentration factor	1.000	3/2/2018 8:29:22 PM	C:\Sirius_T3\KOH18B27.t3r
Acid concentration factor	0.999	3/2/2018 8:29:22 PM	C:\Sirius_T3\HCl18C02.t3r

Instrument Settings

Setting	Value	Batch Id	Install date
Instrument owner	Merck		
Instrument ID	T312060		
Instrument type	T3 Simulator		
Software version	1.1.3.0		
Dispenser module		T3DM1200361	3/31/2009 5:24:52 AM
Dispenser 0	Water		3/31/2009 5:25:05 AM
Syringe volume	2.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Water (0.15 M KCl)	02-06-2018	2/27/2018 10:05:59 AM
Dispenser 2	Acid		3/31/2009 5:25:11 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Acid (0.5 M HCl)	02-27-2018	2/27/2018 10:27:22 AM
Dispenser 1	Base		3/31/2009 5:25:21 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Base (0.5 M KOH)	9/22/2017	2/27/2018 10:21:22 AM
Dispenser 5	Cosolvent		3/31/2009 5:26:24 AM
Syringe volume	2.5 mL		
Firmware version	1.2.1(r2)		
Distribution valve 5	Distribution Valve		3/31/2009 5:28:19 AM
Firmware version	1.1.3		
Port A	Methanol (80%, 0.15 M KCl)	09-26-17	2/7/2018 9:42:01 AM
Port B	Cyclohexane	11-01-17	2/27/2018 10:37:57 AM
Dispenser 3	Buffer		8/3/2010 5:05:16 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Dodecane	2018/01/31	2/28/2018 10:18:04 AM
Dispenser 6	Octanol		10/22/2010 10:52:43 AM

Sample name: **M08_octanol**　　　　　　　　　　　Experiment start time: **3/2/2018 8:29:22 PM**
Assay name: **pH-metric high logP**　　　　　　　　　Analyst: **Pion**
Assay ID: **18C-02009**　　　　　　　　　　　　　　Instrument ID: **T312060**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02009_M08_octanol_pH-metric high logP.t3r**

Instrument Settings (continued)

Setting	Value	Batch Id	Install date
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Octanol	01-31-2018	2/27/2018 9:59:35 AM
Titrator		T3TM1200161	3/31/2009 5:24:17 AM
Horizontal axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Vertical axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Chassis I/O firmware version	1.11 AI1DI0DO4 Norgren I/O		
Probe I/O firmware version	1.1.1		
Electrode	T3 Electrode	T3E0923	1/23/2018 2:01:00 PM
E0 calibration	+3.76 mV		3/2/2018 8:29:50 PM
Filling solution	3M KCl	KCL097	3/2/2018 9:43:24 AM
Liquids			
Wash 1	50% IPA:50% Water		3/2/2018 9:45:12 AM
Wash 2	0.5% Trition X-100 in H20		3/2/2018 9:45:15 AM
Buffer position 1	pH7 Wash		3/2/2018 9:45:18 AM
Buffer position 2	pH 7		3/2/2018 9:45:21 AM
Storage position			3/2/2018 9:44:44 AM
Wash water	7.3e+003 mL	02-27-2018	2/27/2018 9:54:39 AM
Waste	8.2e+003 mL		11/28/2017 10:36:29 AM
Temperature controller			8/5/2010 6:35:13 AM
Turbidity detector			3/31/2009 5:24:45 AM
Spectrometer		074811	11/23/2010 11:22:28 AM
Dip probe		10196	
Wavelength coefficient A0	183.333		
Wavelength coefficient A1	2.21568		
Wavelength coefficient A2	-0.000289308		
Total lamp lit time	120:41:49		11/23/2010 11:22:28 AM
Calibrated on	2/27/2018 10:40:38 AM		
Integration time	40		
Scans averaged	10		
Autoloader		T3AL1200345	11/10/2015 9:34:13 AM
Left-right axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Front-back axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Vertical axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Chassis I/O firmware version	1.11 AI1DI0DO4 Norgren I/O		
Configuration			
Alternate titration position	Titration position		
Alternate reference position	Reference position		
Maximum standard vial volume	3.50 mL		
Maximum alternate vial volume	25.00 mL		
Automatic action idle period	5 minute(s)		
Titrant tube volume	1.3 mL		
Syringe flush count	3.50		
Flowing wash pump volume	20.0 mL		
Flowing wash stir duration	5 s		
Flowing wash stir speed	30%		
Solvent wash stir duration	5 s		
Solvent wash stir speed	30%		
Surfactant wash stir duration	5 s		
Surfactant wash stir speed	30%		
E0 calibration minimum number of points	10		
E0 calibration maximum standard deviation	0.01500		
E0 calibration timeout period	60 s		
E0 calibration stir duration	5 s		
E0 calibration preparation stir speed	30%		
E0 calibration buffer wash stir duration	5 s		
E0 calibration buffer wash stir speed	30%		
E0 calibration reading stir speed	0%		

Sample name: **M08_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-02009**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02009_M08_octanol_pH-metric high logP.t3r**

Experiment start time: **3/2/2018 8:29:22 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Instrument Settings (continued)

Setting	Value	Batch Id	Install date
Spectrometer calibration stir duration	5 s		
Spectrometer calibration stir speed	30%		
Spectrometer calibration wash pump volume	20.0 mL		
Spectrometer calibration wash stir duration	5 s		
Spectrometer calibration wash stir speed	30%		
Overhead dispense height	10000		

Refinement Settings

Setting	Value	Default value
Turbidity detection method	None	None
Turbidity wavelength to assess	500.0 nm	500.0 nm
Turbidity maximum absorbance	0.100	0.100
Turbidity probe threshold	50.00	50.00

Experiment Log

[2:37] Air gap created for Water (0.15 M KCl)
[2:38] Air gap created for Acid (0.5 M HCl)
[2:38] Air gap created for Base (0.5 M KOH)
[2:38] Air gap released for Water (0.15 M KCl)
[2:42] Titrator arm moved over Titration position
[2:42] Titration 1 of 3
[2:42] Adding initial titrants
[2:42] Automatically add 1.50000 mL of water
[3:07] Dispensed 1.500000 mL of Water (0.15 M KCl)
[3:12] Titrator arm moved over Drain
[5:53] Titrator arm moved to Titration position
[5:53] Argon flow rate set to 100
[5:53] Stirrer speed set to 10
[5:59] Initial pH = 5.13
[5:59] Iterative adjust 5.13 -> 10.00
[5:59] pH 5.13 -> 10.00
[6:00] Air gap released for Base (0.5 M KOH)
[6:01] Dispensed 0.006797 mL of Base (0.5 M KOH)
[6:06] Holding pH 10.00
[8:06] Stirrer speed set to 0
[8:06] Stirrer speed set to 50
[8:06] Iterative adjust 11.17 -> 10.00
[8:51] Stirrer speed set to 0
[9:51] Datapoint id 2 collected
[9:51] Stirrer speed set to 50
[9:57] pH 10.75 -> 10.55
[9:57] Using cautious pH adjust
[9:57] Air gap released for Acid (0.5 M HCl)
[9:58] Dispensed 0.000423 mL of Acid (0.5 M HCl)
[10:03] Stepping pH = 10.52
[10:18] Stirrer speed set to 0
[10:53] Datapoint id 3 collected
[10:53] Charge balance equation is out by 49.8%
[10:53] Stirrer speed set to 50
[10:58] pH 10.39 -> 10.19
[10:58] Using cautious pH adjust
[10:58] Dispensed 0.000188 mL of Acid (0.5 M HCl)
[11:03] Stepping pH = 10.34
[11:04] Dispensed 0.000306 mL of Acid (0.5 M HCl)
[11:09] Stepping pH = 10.16
[11:24] Stirrer speed set to 0
[12:04] Datapoint id 4 collected

Sample name: **M08_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-02009**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02009_M08_octanol_pH-metric high logP.t3r**

Experiment start time: **3/2/2018 8:29:22 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[12:04] Charge balance equation is out by -24.4%
[12:04] Stirrer speed set to 50
[12:09] pH 10.05 -> 9.85
[12:09] Using cautious pH adjust
[12:09] Dispensed 0.000094 mL of Acid (0.5 M HCl)
[12:15] Stepping pH = 10.02
[12:15] Dispensed 0.000235 mL of Acid (0.5 M HCl)
[12:20] Stepping pH = 9.77
[12:35] Stirrer speed set to 0
[13:03] Datapoint id 5 collected
[13:03] Charge balance equation is out by -70.9%
[13:03] Stirrer speed set to 50
[13:09] pH 9.66 -> 9.46
[13:09] Using cautious pH adjust
[13:09] Dispensed 0.000047 mL of Acid (0.5 M HCl)
[13:14] Stepping pH = 9.64
[13:14] Dispensed 0.000141 mL of Acid (0.5 M HCl)
[13:19] Stepping pH = 9.39
[13:34] Stirrer speed set to 0
[14:07] Datapoint id 6 collected
[14:07] Charge balance equation is out by -86.9%
[14:07] Stirrer speed set to 50
[14:12] pH 9.28 -> 9.08
[14:12] Using cautious pH adjust
[14:12] Dispensed 0.000024 mL of Acid (0.5 M HCl)
[14:17] Stepping pH = 9.26
[14:17] Dispensed 0.000071 mL of Acid (0.5 M HCl)
[14:22] Stepping pH = 9.10
[14:22] Dispensed 0.000024 mL of Acid (0.5 M HCl)
[14:27] Stepping pH = 9.03
[14:42] Stirrer speed set to 0
[15:18] Datapoint id 7 collected
[15:18] Charge balance equation is out by -126.0%
[15:18] Stirrer speed set to 50
[15:23] pH 8.82 -> 8.62
[15:23] Using cautious pH adjust
[15:23] Dispensed 0.000024 mL of Acid (0.5 M HCl)
[15:28] Stepping pH = 8.78
[15:28] Dispensed 0.000024 mL of Acid (0.5 M HCl)
[15:34] Stepping pH = 8.69
[15:34] Dispensed 0.000024 mL of Acid (0.5 M HCl)
[15:39] Stepping pH = 8.55
[15:54] Stirrer speed set to 0
[16:43] Datapoint id 8 collected
[16:43] Charge balance equation is out by -159.4%
[16:43] Stirrer speed set to 50
[16:48] pH 8.28 -> 8.08
[16:48] Using cautious pH adjust
[16:48] Dispensed 0.000024 mL of Acid (0.5 M HCl)
[16:53] Stepping pH = 8.24
[16:53] Dispensed 0.000024 mL of Acid (0.5 M HCl)
[16:58] Stepping pH = 8.17
[16:58] Dispensed 0.000024 mL of Acid (0.5 M HCl)
[17:03] Stepping pH = 8.08
[17:19] Stirrer speed set to 0
[17:38] Datapoint id 9 collected
[17:38] Charge balance equation is out by -148.3%
[17:38] Stirrer speed set to 50
[17:43] pH 7.95 -> 7.75

Sample name: **M08_octanol**   Experiment start time: **3/2/2018 8:29:22 PM**
Assay name: **pH-metric high logP**   Analyst: **Pion**
Assay ID: **18C-02009**   Instrument ID: **T312060**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02009_M08_octanol_pH-metric high logP.t3r**

Experiment Log (continued)

[17:43] Using cautious pH adjust
[17:43] Dispensed 0.000024 mL of Acid (0.5 M HCl)
[17:48] Stepping pH = 7.92
[17:48] Dispensed 0.000071 mL of Acid (0.5 M HCl)
[17:53] Stepping pH = 7.72
[18:09] Stirrer speed set to 0
[18:26] Datapoint id 10 collected
[18:26] Charge balance equation is out by -62.6%
[18:26] Stirrer speed set to 50
[18:31] pH 7.65 -> 7.45
[18:31] Using cautious pH adjust
[18:31] Dispensed 0.000047 mL of Acid (0.5 M HCl)
[18:36] Stepping pH = 7.62
[18:36] Dispensed 0.000094 mL of Acid (0.5 M HCl)
[18:41] Stepping pH = 7.44
[18:56] Stirrer speed set to 0
[19:13] Datapoint id 11 collected
[19:13] Charge balance equation is out by -49.6%
[19:13] Stirrer speed set to 50
[19:18] pH 7.42 -> 7.22
[19:18] Using cautious pH adjust
[19:18] Dispensed 0.000071 mL of Acid (0.5 M HCl)
[19:23] Stepping pH = 7.36
[19:23] Dispensed 0.000094 mL of Acid (0.5 M HCl)
[19:29] Stepping pH = 7.25
[19:29] Dispensed 0.000024 mL of Acid (0.5 M HCl)
[19:34] Stepping pH = 7.24
[19:34] Dispensed 0.000047 mL of Acid (0.5 M HCl)
[19:39] Stepping pH = 7.21
[19:54] Stirrer speed set to 0
[20:15] Datapoint id 12 collected
[20:15] Charge balance equation is out by -60.4%
[20:15] Stirrer speed set to 50
[20:20] pH 7.21 -> 7.01
[20:20] Using cautious pH adjust
[20:20] Dispensed 0.000118 mL of Acid (0.5 M HCl)
[20:25] Stepping pH = 7.11
[20:25] Dispensed 0.000094 mL of Acid (0.5 M HCl)
[20:30] Stepping pH = 7.04
[20:31] Dispensed 0.000047 mL of Acid (0.5 M HCl)
[20:36] Stepping pH = 7.03
[20:36] Dispensed 0.000047 mL of Acid (0.5 M HCl)
[20:41] Stepping pH = 7.01
[20:56] Stirrer speed set to 0
[21:13] Datapoint id 13 collected
[21:13] Charge balance equation is out by -27.4%
[21:13] Stirrer speed set to 50
[21:18] pH 7.02 -> 6.82
[21:18] Using cautious pH adjust
[21:18] Dispensed 0.000165 mL of Acid (0.5 M HCl)
[21:23] Stepping pH = 6.90
[21:23] Dispensed 0.000094 mL of Acid (0.5 M HCl)
[21:28] Stepping pH = 6.86
[21:28] Dispensed 0.000071 mL of Acid (0.5 M HCl)
[21:34] Stepping pH = 6.84
[21:34] Dispensed 0.000071 mL of Acid (0.5 M HCl)
[21:39] Stepping pH = 6.82
[21:54] Stirrer speed set to 0
[22:10] Datapoint id 14 collected

Sample name: **M08_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-02009**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02009_M08_octanol_pH-metric high logP.t3r**

Experiment start time: **3/2/2018 8:29:22 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[22:10] Charge balance equation is out by -25.3%
[22:10] Stirrer speed set to 50
[22:15] pH 6.84 -> 6.64
[22:15] Using cautious pH adjust
[22:15] Dispensed 0.000235 mL of Acid (0.5 M HCl)
[22:20] Stepping pH = 6.72
[22:20] Dispensed 0.000118 mL of Acid (0.5 M HCl)
[22:25] Stepping pH = 6.68
[22:25] Dispensed 0.000094 mL of Acid (0.5 M HCl)
[22:30] Stepping pH = 6.66
[22:30] Dispensed 0.000071 mL of Acid (0.5 M HCl)
[22:36] Stepping pH = 6.65
[22:51] Stirrer speed set to 0
[23:07] Datapoint id 15 collected
[23:07] Charge balance equation is out by -11.8%
[23:07] Stirrer speed set to 50
[23:12] pH 6.67 -> 6.47
[23:12] Using charge balance adjust
[23:12] Dispensed 0.000564 mL of Acid (0.5 M HCl)
[23:33] Stirrer speed set to 0
[23:50] Datapoint id 16 collected
[23:50] Charge balance equation is out by -18.0%
[23:50] Stirrer speed set to 50
[23:55] pH 6.50 -> 6.30
[23:55] Using cautious pH adjust
[23:55] Dispensed 0.000329 mL of Acid (0.5 M HCl)
[24:00] Stepping pH = 6.39
[24:00] Dispensed 0.000212 mL of Acid (0.5 M HCl)
[24:05] Stepping pH = 6.35
[24:05] Dispensed 0.000165 mL of Acid (0.5 M HCl)
[24:10] Stepping pH = 6.32
[24:10] Dispensed 0.000071 mL of Acid (0.5 M HCl)
[24:15] Stepping pH = 6.32
[24:15] Dispensed 0.000212 mL of Acid (0.5 M HCl)
[24:21] Stepping pH = 6.26
[24:36] Stirrer speed set to 0
[24:49] Datapoint id 17 collected
[24:49] Charge balance equation is out by -45.8%
[24:49] Stirrer speed set to 50
[24:54] pH 6.29 -> 6.09
[24:54] Using cautious pH adjust
[24:54] Dispensed 0.000400 mL of Acid (0.5 M HCl)
[25:00] Stepping pH = 6.17
[25:00] Dispensed 0.000212 mL of Acid (0.5 M HCl)
[25:05] Stepping pH = 6.13
[25:05] Dispensed 0.000165 mL of Acid (0.5 M HCl)
[25:10] Stepping pH = 6.10
[25:25] Stirrer speed set to 0
[25:38] Datapoint id 18 collected
[25:38] Charge balance equation is out by 3.6%
[25:38] Stirrer speed set to 50
[25:44] pH 6.12 -> 5.92
[25:44] Using charge balance adjust
[25:44] Dispensed 0.000800 mL of Acid (0.5 M HCl)
[26:04] Stirrer speed set to 0
[26:16] Datapoint id 19 collected
[26:16] Charge balance equation is out by 1.0%
[26:16] Stirrer speed set to 50
[26:22] pH 5.92 -> 5.72

Sample name: **M08_octanol** Experiment start time: **3/2/2018 8:29:22 PM**
Assay name: **pH-metric high logP** Analyst: **Pion**
Assay ID: **18C-02009** Instrument ID: **T312060**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02009_M08_octanol_pH-metric high logP.t3r**

Experiment Log (continued)

[26:22] Using charge balance adjust
[26:22] Dispensed 0.000753 mL of Acid (0.5 M HCl)
[26:42] Stirrer speed set to 0
[26:58] Datapoint id 20 collected
[26:58] Charge balance equation is out by 4.1%
[26:58] Stirrer speed set to 50
[27:03] pH 5.71 -> 5.51
[27:03] Using charge balance adjust
[27:03] Dispensed 0.000635 mL of Acid (0.5 M HCl)
[27:23] Stirrer speed set to 0
[27:40] Datapoint id 21 collected
[27:40] Charge balance equation is out by 17.0%
[27:40] Stirrer speed set to 50
[27:45] pH 5.48 -> 5.28
[27:45] Using cautious pH adjust
[27:45] Dispensed 0.000235 mL of Acid (0.5 M HCl)
[27:51] Stepping pH = 5.37
[27:51] Dispensed 0.000141 mL of Acid (0.5 M HCl)
[27:56] Stepping pH = 5.29
[27:56] Dispensed 0.000024 mL of Acid (0.5 M HCl)
[28:01] Stepping pH = 5.30
[28:01] Dispensed 0.000165 mL of Acid (0.5 M HCl)
[28:06] Stepping pH = 5.18
[28:21] Stirrer speed set to 0
[28:42] Datapoint id 22 collected
[28:42] Charge balance equation is out by -22.3%
[28:42] Stirrer speed set to 50
[28:47] pH 5.18 -> 4.98
[28:47] Using cautious pH adjust
[28:47] Dispensed 0.000141 mL of Acid (0.5 M HCl)
[28:52] Stepping pH = 5.08
[28:52] Dispensed 0.000094 mL of Acid (0.5 M HCl)
[28:58] Stepping pH = 4.98
[29:13] Stirrer speed set to 0
[30:13] Datapoint id 23 collected
[30:13] Charge balance equation is out by 20.1%
[30:13] Stirrer speed set to 50
[30:18] pH 5.05 -> 4.85
[30:18] Using cautious pH adjust
[30:18] Dispensed 0.000118 mL of Acid (0.5 M HCl)
[30:23] Stepping pH = 4.93
[30:23] Dispensed 0.000047 mL of Acid (0.5 M HCl)
[30:28] Stepping pH = 4.88
[30:28] Dispensed 0.000024 mL of Acid (0.5 M HCl)
[30:33] Stepping pH = 4.87
[30:33] Dispensed 0.000024 mL of Acid (0.5 M HCl)
[30:38] Stepping pH = 4.83
[30:53] Stirrer speed set to 0
[31:53] Datapoint id 24 collected
[31:53] Charge balance equation is out by 5.3%
[31:53] Stirrer speed set to 50
[31:59] pH 4.99 -> 4.79
[31:59] Using charge balance adjust
[31:59] Dispensed 0.000212 mL of Acid (0.5 M HCl)
[32:19] Stirrer speed set to 0
[32:52] Datapoint id 25 collected
[32:52] Charge balance equation is out by 145.5%
[32:52] Stirrer speed set to 50
[32:57] pH 4.51 -> 4.31

Sample name: **M08_octanol**   Experiment start time: **3/2/2018 8:29:22 PM**
Assay name: **pH-metric high logP**   Analyst: **Pion**
Assay ID: **18C-02009**   Instrument ID: **T312060**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02009_M08_octanol_pH-metric high logP.t3r**

Experiment Log (continued)

[32:57] Using cautious pH adjust
[32:57] Dispensed 0.000071 mL of Acid (0.5 M HCl)
[33:02] Stepping pH = 4.40
[33:02] Dispensed 0.000047 mL of Acid (0.5 M HCl)
[33:07] Stepping pH = 4.32
[33:22] Stirrer speed set to 0
[33:48] Datapoint id 26 collected
[33:48] Charge balance equation is out by 19.0%
[33:48] Stirrer speed set to 50
[33:53] pH 4.31 -> 4.11
[33:53] Using cautious pH adjust
[33:53] Dispensed 0.000071 mL of Acid (0.5 M HCl)
[33:58] Stepping pH = 4.21
[33:58] Dispensed 0.000047 mL of Acid (0.5 M HCl)
[34:03] Stepping pH = 4.14
[34:03] Dispensed 0.000024 mL of Acid (0.5 M HCl)
[34:08] Stepping pH = 4.12
[34:24] Stirrer speed set to 0
[34:34] Datapoint id 27 collected
[34:34] Charge balance equation is out by 1.1%
[34:34] Stirrer speed set to 50
[34:39] pH 4.11 -> 3.91
[34:39] Using charge balance adjust
[34:39] Dispensed 0.000212 mL of Acid (0.5 M HCl)
[34:59] Stirrer speed set to 0
[35:09] Datapoint id 28 collected
[35:10] Charge balance equation is out by 21.2%
[35:10] Stirrer speed set to 50
[35:15] pH 3.87 -> 3.67
[35:15] Using cautious pH adjust
[35:15] Dispensed 0.000165 mL of Acid (0.5 M HCl)
[35:20] Stepping pH = 3.76
[35:20] Dispensed 0.000094 mL of Acid (0.5 M HCl)
[35:25] Stepping pH = 3.71
[35:25] Dispensed 0.000047 mL of Acid (0.5 M HCl)
[35:30] Stepping pH = 3.69
[35:30] Dispensed 0.000047 mL of Acid (0.5 M HCl)
[35:35] Stepping pH = 3.67
[35:50] Stirrer speed set to 0
[36:00] Datapoint id 29 collected
[36:00] Charge balance equation is out by -14.5%
[36:00] Stirrer speed set to 50
[36:05] pH 3.67 -> 3.47
[36:05] Using charge balance adjust
[36:06] Dispensed 0.000494 mL of Acid (0.5 M HCl)
[36:26] Stirrer speed set to 0
[36:36] Datapoint id 30 collected
[36:36] Charge balance equation is out by 10.8%
[36:36] Stirrer speed set to 50
[36:41] pH 3.45 -> 3.25
[36:41] Using charge balance adjust
[36:41] Dispensed 0.000800 mL of Acid (0.5 M HCl)
[37:02] Stirrer speed set to 0
[37:12] Datapoint id 31 collected
[37:12] Charge balance equation is out by 0.6%
[37:12] Stirrer speed set to 50
[37:17] pH 3.26 -> 3.06
[37:17] Using charge balance adjust
[37:17] Dispensed 0.001270 mL of Acid (0.5 M HCl)

Sample name: **M08_octanol** Experiment start time: **3/2/2018 8:29:22 PM**
Assay name: **pH-metric high logP** Analyst: **Pion**
Assay ID: **18C-02009** Instrument ID: **T312060**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02009_M08_octanol_pH-metric high logP.t3r**

Experiment Log (continued)

[37:37] Stirrer speed set to 0
[37:47] Datapoint id 32 collected
[37:47] Charge balance equation is out by -2.6%
[37:47] Stirrer speed set to 50
[37:52] pH 3.07 -> 2.87
[37:52] Using charge balance adjust
[37:52] Dispensed 0.001952 mL of Acid (0.5 M HCl)
[38:13] Stirrer speed set to 0
[38:23] Datapoint id 33 collected
[38:23] Charge balance equation is out by -7.9%
[38:23] Stirrer speed set to 50
[38:28] pH 2.89 -> 2.69
[38:28] Using charge balance adjust
[38:28] Dispensed 0.002963 mL of Acid (0.5 M HCl)
[38:48] Stirrer speed set to 0
[38:58] Datapoint id 34 collected
[38:58] Charge balance equation is out by -8.0%
[38:58] Stirrer speed set to 50
[39:03] pH 2.71 -> 2.51
[39:03] Using charge balance adjust
[39:04] Dispensed 0.004492 mL of Acid (0.5 M HCl)
[39:24] Stirrer speed set to 0
[39:34] Datapoint id 35 collected
[39:34] Charge balance equation is out by -8.4%
[39:34] Stirrer speed set to 50
[39:39] pH 2.54 -> 2.34
[39:39] Using charge balance adjust
[39:39] Dispensed 0.006844 mL of Acid (0.5 M HCl)
[39:59] Stirrer speed set to 0
[40:09] Datapoint id 36 collected
[40:09] Charge balance equation is out by -3.3%
[40:09] Stirrer speed set to 50
[40:15] pH 2.35 -> 2.15
[40:15] Using charge balance adjust
[40:15] Dispensed 0.010724 mL of Acid (0.5 M HCl)
[40:35] Stirrer speed set to 0
[40:45] Datapoint id 37 collected
[40:45] Charge balance equation is out by -4.4%
[40:45] Stirrer speed set to 50
[40:50] pH 2.16 -> 1.96
[40:50] Using charge balance adjust
[40:51] Dispensed 0.016886 mL of Acid (0.5 M HCl)
[41:11] Stirrer speed set to 0
[41:22] Datapoint id 38 collected
[41:22] Charge balance equation is out by -3.8%
[41:22] Titration 2 of 3
[41:22] Adding initial titrants
[41:22] Automatically add 0.20000 mL of Octanol
[41:26] Dispensed 0.200000 mL of Octanol
[41:26] Stirrer speed set to 10
[41:27] Stirrer speed set to 55
[41:27] Iterative adjust 1.97 -> 10.00
[41:27] pH 1.97 -> 10.00
[41:29] Dispensed 0.051670 mL of Base (0.5 M KOH)
[42:19] Stirrer speed set to 0
[43:19] Datapoint id 39 collected
[43:19] Stirrer speed set to 55
[43:24] pH 7.36 -> 7.16
[43:24] Using cautious pH adjust

Sample name: **M08_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-02009**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02009_M08_octanol_pH-metric high logP.t3r**

Experiment start time: **3/2/2018 8:29:22 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[43:24] Dispensed 0.000212 mL of Acid (0.5 M HCl)
[43:29] Stepping pH = 7.24
[43:29] Dispensed 0.000118 mL of Acid (0.5 M HCl)
[43:34] Stepping pH = 7.17
[43:49] Stirrer speed set to 0
[44:26] Datapoint id 40 collected
[44:26] Charge balance equation is out by 21.6%
[44:26] Stirrer speed set to 55
[44:31] pH 7.10 -> 6.90
[44:31] Using cautious pH adjust
[44:31] Dispensed 0.000306 mL of Acid (0.5 M HCl)
[44:36] Stepping pH = 6.94
[44:36] Dispensed 0.000094 mL of Acid (0.5 M HCl)
[44:41] Stepping pH = 6.93
[44:42] Dispensed 0.000094 mL of Acid (0.5 M HCl)
[44:47] Stepping pH = 6.89
[45:02] Stirrer speed set to 0
[45:23] Datapoint id 41 collected
[45:23] Charge balance equation is out by 21.8%
[45:23] Stirrer speed set to 55
[45:28] pH 6.89 -> 6.69
[45:28] Using cautious pH adjust
[45:28] Dispensed 0.000376 mL of Acid (0.5 M HCl)
[45:33] Stepping pH = 6.72
[45:33] Dispensed 0.000047 mL of Acid (0.5 M HCl)
[45:38] Stepping pH = 6.74
[45:38] Dispensed 0.000447 mL of Acid (0.5 M HCl)
[45:43] Stepping pH = 6.56
[45:58] Stirrer speed set to 0
[46:25] Datapoint id 42 collected
[46:25] Charge balance equation is out by -19.0%
[46:25] Stirrer speed set to 55
[46:30] pH 6.59 -> 6.39
[46:30] Using cautious pH adjust
[46:30] Dispensed 0.000400 mL of Acid (0.5 M HCl)
[46:35] Stepping pH = 6.44
[46:35] Dispensed 0.000141 mL of Acid (0.5 M HCl)
[46:40] Stepping pH = 6.41
[46:41] Dispensed 0.000071 mL of Acid (0.5 M HCl)
[46:46] Stepping pH = 6.39
[47:01] Stirrer speed set to 0
[47:28] Datapoint id 43 collected
[47:28] Charge balance equation is out by 24.6%
[47:28] Stirrer speed set to 55
[47:33] pH 6.41 -> 6.21
[47:33] Using cautious pH adjust
[47:33] Dispensed 0.000376 mL of Acid (0.5 M HCl)
[47:38] Stepping pH = 6.25
[47:38] Dispensed 0.000071 mL of Acid (0.5 M HCl)
[47:43] Stepping pH = 6.24
[47:43] Dispensed 0.000071 mL of Acid (0.5 M HCl)
[47:48] Stepping pH = 6.21
[48:03] Stirrer speed set to 0
[48:29] Datapoint id 44 collected
[48:29] Charge balance equation is out by 30.2%
[48:29] Stirrer speed set to 55
[48:34] pH 6.24 -> 6.04
[48:34] Using cautious pH adjust
[48:34] Dispensed 0.000329 mL of Acid (0.5 M HCl)

Sample name: **M08_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-02009**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02009_M08_octanol_pH-metric high logP.t3r**

Experiment start time: **3/2/2018 8:29:22 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[48:39] Stepping pH = 6.06
[48:39] Dispensed 0.000047 mL of Acid (0.5 M HCl)
[48:44] Stepping pH = 6.06
[48:44] Dispensed 0.000071 mL of Acid (0.5 M HCl)
[48:49] Stepping pH = 6.02
[49:04] Stirrer speed set to 0
[49:31] Datapoint id 45 collected
[49:31] Charge balance equation is out by 32.8%
[49:31] Stirrer speed set to 55
[49:36] pH 6.04 -> 5.84
[49:36] Using cautious pH adjust
[49:36] Dispensed 0.000259 mL of Acid (0.5 M HCl)
[49:41] Stepping pH = 5.87
[49:41] Dispensed 0.000024 mL of Acid (0.5 M HCl)
[49:46] Stepping pH = 5.86
[49:46] Dispensed 0.000071 mL of Acid (0.5 M HCl)
[49:51] Stepping pH = 5.82
[50:06] Stirrer speed set to 0
[50:28] Datapoint id 46 collected
[50:28] Charge balance equation is out by 30.4%
[50:28] Stirrer speed set to 55
[50:34] pH 5.85 -> 5.65
[50:34] Using cautious pH adjust
[50:34] Dispensed 0.000188 mL of Acid (0.5 M HCl)
[50:39] Stepping pH = 5.67
[50:39] Dispensed 0.000024 mL of Acid (0.5 M HCl)
[50:44] Stepping pH = 5.68
[50:44] Dispensed 0.000165 mL of Acid (0.5 M HCl)
[50:49] Stepping pH = 5.46
[51:04] Stirrer speed set to 0
[51:23] Datapoint id 47 collected
[51:23] Charge balance equation is out by 5.3%
[51:23] Stirrer speed set to 55
[51:28] pH 5.48 -> 5.28
[51:28] Using charge balance adjust
[51:28] Dispensed 0.000212 mL of Acid (0.5 M HCl)
[51:49] Stirrer speed set to 0
[52:05] Datapoint id 48 collected
[52:05] Charge balance equation is out by 71.8%
[52:05] Stirrer speed set to 55
[52:10] pH 5.12 -> 4.92
[52:10] Using cautious pH adjust
[52:10] Dispensed 0.000047 mL of Acid (0.5 M HCl)
[52:15] Stepping pH = 5.10
[52:15] Dispensed 0.000165 mL of Acid (0.5 M HCl)
[52:21] Stepping pH = 4.66
[52:36] Stirrer speed set to 0
[52:52] Datapoint id 49 collected
[52:52] Charge balance equation is out by -86.2%
[52:52] Stirrer speed set to 55
[52:57] pH 4.66 -> 4.46
[52:57] Using cautious pH adjust
[52:57] Dispensed 0.000047 mL of Acid (0.5 M HCl)
[53:02] Stepping pH = 4.65
[53:02] Dispensed 0.000118 mL of Acid (0.5 M HCl)
[53:07] Stepping pH = 4.41
[53:22] Stirrer speed set to 0
[53:34] Datapoint id 50 collected
[53:34] Charge balance equation is out by -89.3%

Sample name: **M08_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-02009**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02009_M08_octanol_pH-metric high logP.t3r**

Experiment start time: **3/2/2018 8:29:22 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[53:34] Stirrer speed set to 55
[53:39] pH 4.40 -> 4.20
[53:39] Using cautious pH adjust
[53:39] Dispensed 0.000047 mL of Acid (0.5 M HCl)
[53:44] Stepping pH = 4.39
[53:44] Dispensed 0.000165 mL of Acid (0.5 M HCl)
[53:49] Stepping pH = 4.17
[54:04] Stirrer speed set to 0
[54:15] Datapoint id 51 collected
[54:15] Charge balance equation is out by -92.5%
[54:15] Stirrer speed set to 55
[54:20] pH 4.17 -> 3.97
[54:20] Using cautious pH adjust
[54:20] Dispensed 0.000094 mL of Acid (0.5 M HCl)
[54:25] Stepping pH = 4.12
[54:25] Dispensed 0.000118 mL of Acid (0.5 M HCl)
[54:30] Stepping pH = 3.99
[54:30] Dispensed 0.000024 mL of Acid (0.5 M HCl)
[54:35] Stepping pH = 3.98
[54:50] Stirrer speed set to 0
[55:00] Datapoint id 52 collected
[55:00] Charge balance equation is out by -30.4%
[55:00] Stirrer speed set to 55
[55:06] pH 3.98 -> 3.78
[55:06] Using cautious pH adjust
[55:06] Dispensed 0.000141 mL of Acid (0.5 M HCl)
[55:11] Stepping pH = 3.89
[55:11] Dispensed 0.000118 mL of Acid (0.5 M HCl)
[55:16] Stepping pH = 3.82
[55:16] Dispensed 0.000047 mL of Acid (0.5 M HCl)
[55:21] Stepping pH = 3.80
[55:21] Dispensed 0.000047 mL of Acid (0.5 M HCl)
[55:26] Stepping pH = 3.78
[55:41] Stirrer speed set to 0
[55:51] Datapoint id 53 collected
[55:51] Charge balance equation is out by -27.9%
[55:51] Stirrer speed set to 55
[55:56] pH 3.78 -> 3.58
[55:56] Using cautious pH adjust
[55:56] Dispensed 0.000212 mL of Acid (0.5 M HCl)
[56:02] Stepping pH = 3.67
[56:02] Dispensed 0.000141 mL of Acid (0.5 M HCl)
[56:07] Stepping pH = 3.62
[56:07] Dispensed 0.000094 mL of Acid (0.5 M HCl)
[56:12] Stepping pH = 3.59
[56:12] Dispensed 0.000024 mL of Acid (0.5 M HCl)
[56:17] Stepping pH = 3.59
[56:32] Stirrer speed set to 0
[56:42] Datapoint id 54 collected
[56:42] Charge balance equation is out by -15.7%
[56:42] Stirrer speed set to 55
[56:47] pH 3.59 -> 3.39
[56:47] Using cautious pH adjust
[56:47] Dispensed 0.000306 mL of Acid (0.5 M HCl)
[56:52] Stepping pH = 3.50
[56:53] Dispensed 0.000282 mL of Acid (0.5 M HCl)
[56:58] Stepping pH = 3.41
[56:58] Dispensed 0.000071 mL of Acid (0.5 M HCl)
[57:03] Stepping pH = 3.40

Sample name: **M08_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-02009**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02009_M08_octanol_pH-metric high logP.t3r**

Experiment start time: **3/2/2018 8:29:22 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[57:03] Dispensed 0.000094 mL of Acid (0.5 M HCl)
[57:08] Stepping pH = 3.38
[57:23] Stirrer speed set to 0
[57:33] Datapoint id 55 collected
[57:33] Charge balance equation is out by -22.9%
[57:33] Stirrer speed set to 55
[57:38] pH 3.38 -> 3.18
[57:38] Using cautious pH adjust
[57:38] Dispensed 0.000517 mL of Acid (0.5 M HCl)
[57:43] Stepping pH = 3.26
[57:43] Dispensed 0.000282 mL of Acid (0.5 M HCl)
[57:49] Stepping pH = 3.21
[57:49] Dispensed 0.000165 mL of Acid (0.5 M HCl)
[57:54] Stepping pH = 3.19
[58:09] Stirrer speed set to 0
[58:19] Datapoint id 56 collected
[58:19] Charge balance equation is out by 5.3%
[58:19] Stirrer speed set to 55
[58:24] pH 3.19 -> 2.99
[58:24] Using charge balance adjust
[58:24] Dispensed 0.001576 mL of Acid (0.5 M HCl)
[58:44] Stirrer speed set to 0
[58:54] Datapoint id 57 collected
[58:54] Charge balance equation is out by -0.7%
[58:54] Stirrer speed set to 55
[58:59] pH 3.00 -> 2.80
[58:59] Using charge balance adjust
[59:00] Dispensed 0.002469 mL of Acid (0.5 M HCl)
[59:20] Stirrer speed set to 0
[59:30] Datapoint id 58 collected
[59:30] Charge balance equation is out by -1.6%
[59:30] Stirrer speed set to 55
[59:35] pH 2.81 -> 2.61
[59:35] Using charge balance adjust
[59:35] Dispensed 0.003881 mL of Acid (0.5 M HCl)
[59:55] Stirrer speed set to 0
[1:00:05] Datapoint id 59 collected
[1:00:05] Charge balance equation is out by -2.2%
[1:00:05] Stirrer speed set to 55
[1:00:10] pH 2.61 -> 2.41
[1:00:10] Using charge balance adjust
[1:00:11] Dispensed 0.006091 mL of Acid (0.5 M HCl)
[1:00:31] Stirrer speed set to 0
[1:00:41] Datapoint id 60 collected
[1:00:41] Charge balance equation is out by -0.3%
[1:00:41] Stirrer speed set to 55
[1:00:46] pH 2.42 -> 2.22
[1:00:46] Using charge balance adjust
[1:00:46] Dispensed 0.009690 mL of Acid (0.5 M HCl)
[1:01:07] Stirrer speed set to 0
[1:01:17] Datapoint id 61 collected
[1:01:17] Charge balance equation is out by -8.4%
[1:01:17] Stirrer speed set to 55
[1:01:22] pH 2.24 -> 2.04
[1:01:22] Using charge balance adjust
[1:01:22] Dispensed 0.014981 mL of Acid (0.5 M HCl)
[1:01:42] Stirrer speed set to 0
[1:01:52] Datapoint id 62 collected
[1:01:52] Charge balance equation is out by -3.3%

Sample name: **M08_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-02009**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02009_M08_octanol_pH-metric high logP.t3r**

Experiment start time: **3/2/2018 8:29:22 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[1:01:52] Stirrer speed set to 55
[1:01:58] pH 2.05 -> 1.95
[1:01:58] Using charge balance adjust
[1:01:58] Dispensed 0.010395 mL of Acid (0.5 M HCl)
[1:02:18] Stirrer speed set to 0
[1:02:28] Datapoint id 63 collected
[1:02:28] Charge balance equation is out by -51.4%
[1:02:28] Titration 3 of 3
[1:02:28] Adding initial titrants
[1:02:28] Automatically add 0.80000 mL of Octanol
[1:03:18] Dispensed 0.800000 mL of Octanol
[1:03:18] Stirrer speed set to 10
[1:03:19] Stirrer speed set to 60
[1:03:19] Iterative adjust 1.94 -> 10.00
[1:03:19] pH 1.94 -> 10.00
[1:03:21] Dispensed 0.058137 mL of Base (0.5 M KOH)
[1:04:11] Stirrer speed set to 0
[1:05:11] Datapoint id 64 collected
[1:05:11] Stirrer speed set to 60
[1:05:16] pH 8.61 -> 8.41
[1:05:16] Using cautious pH adjust
[1:05:16] Dispensed 0.000071 mL of Acid (0.5 M HCl)
[1:05:21] Stepping pH = 8.48
[1:05:21] Dispensed 0.000024 mL of Acid (0.5 M HCl)
[1:05:26] Stepping pH = 8.35
[1:05:42] Stirrer speed set to 0
[1:06:42] Datapoint id 65 collected
[1:06:42] Charge balance equation is out by 28.7%
[1:06:42] Stirrer speed set to 60
[1:06:47] pH 7.80 -> 7.60
[1:06:47] Using cautious pH adjust
[1:06:47] Dispensed 0.000259 mL of Acid (0.5 M HCl)
[1:06:52] Stepping pH = 7.65
[1:06:52] Dispensed 0.000071 mL of Acid (0.5 M HCl)
[1:06:57] Stepping pH = 7.62
[1:06:57] Dispensed 0.000047 mL of Acid (0.5 M HCl)
[1:07:02] Stepping pH = 7.60
[1:07:17] Stirrer speed set to 0
[1:07:38] Datapoint id 66 collected
[1:07:38] Charge balance equation is out by 24.0%
[1:07:38] Stirrer speed set to 60
[1:07:43] pH 7.54 -> 7.34
[1:07:43] Using cautious pH adjust
[1:07:43] Dispensed 0.000329 mL of Acid (0.5 M HCl)
[1:07:48] Stepping pH = 7.40
[1:07:48] Dispensed 0.000141 mL of Acid (0.5 M HCl)
[1:07:53] Stepping pH = 7.36
[1:07:53] Dispensed 0.000047 mL of Acid (0.5 M HCl)
[1:07:58] Stepping pH = 7.35
[1:08:13] Stirrer speed set to 0
[1:08:39] Datapoint id 67 collected
[1:08:39] Charge balance equation is out by 23.3%
[1:08:39] Stirrer speed set to 60
[1:08:44] pH 7.32 -> 7.12
[1:08:44] Using cautious pH adjust
[1:08:44] Dispensed 0.000400 mL of Acid (0.5 M HCl)
[1:08:49] Stepping pH = 7.18
[1:08:49] Dispensed 0.000165 mL of Acid (0.5 M HCl)
[1:08:54] Stepping pH = 7.14

Sample name: **M08_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-02009**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02009_M08_octanol_pH-metric high logP.t3r**

Experiment start time: **3/2/2018 8:29:22 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[1:08:54] Dispensed 0.000071 mL of Acid (0.5 M HCl)
[1:08:59] Stepping pH = 7.12
[1:09:14] Stirrer speed set to 0
[1:09:39] Datapoint id 68 collected
[1:09:39] Charge balance equation is out by 21.8%
[1:09:39] Stirrer speed set to 60
[1:09:44] pH 7.11 -> 6.91
[1:09:44] Using cautious pH adjust
[1:09:44] Dispensed 0.000400 mL of Acid (0.5 M HCl)
[1:09:49] Stepping pH = 6.98
[1:09:49] Dispensed 0.000165 mL of Acid (0.5 M HCl)
[1:09:54] Stepping pH = 6.94
[1:09:54] Dispensed 0.000094 mL of Acid (0.5 M HCl)
[1:09:59] Stepping pH = 6.92
[1:10:15] Stirrer speed set to 0
[1:10:46] Datapoint id 69 collected
[1:10:46] Charge balance equation is out by 16.7%
[1:10:46] Stirrer speed set to 60
[1:10:51] pH 6.92 -> 6.72
[1:10:51] Using cautious pH adjust
[1:10:51] Dispensed 0.000376 mL of Acid (0.5 M HCl)
[1:10:56] Stepping pH = 6.79
[1:10:56] Dispensed 0.000165 mL of Acid (0.5 M HCl)
[1:11:02] Stepping pH = 6.74
[1:11:02] Dispensed 0.000071 mL of Acid (0.5 M HCl)
[1:11:07] Stepping pH = 6.73
[1:11:07] Dispensed 0.000071 mL of Acid (0.5 M HCl)
[1:11:12] Stepping pH = 6.71
[1:11:27] Stirrer speed set to 0
[1:11:59] Datapoint id 70 collected
[1:11:59] Charge balance equation is out by 9.2%
[1:11:59] Stirrer speed set to 60
[1:12:04] pH 6.71 -> 6.51
[1:12:04] Using charge balance adjust
[1:12:04] Dispensed 0.000611 mL of Acid (0.5 M HCl)
[1:12:24] Stirrer speed set to 0
[1:13:09] Datapoint id 71 collected
[1:13:09] Charge balance equation is out by -12.8%
[1:13:09] Stirrer speed set to 60
[1:13:14] pH 6.46 -> 6.26
[1:13:14] Using charge balance adjust
[1:13:14] Dispensed 0.000447 mL of Acid (0.5 M HCl)
[1:13:34] Stirrer speed set to 0
[1:14:15] Datapoint id 72 collected
[1:14:15] Charge balance equation is out by -34.1%
[1:14:15] Stirrer speed set to 60
[1:14:20] pH 6.25 -> 6.05
[1:14:20] Using cautious pH adjust
[1:14:20] Dispensed 0.000165 mL of Acid (0.5 M HCl)
[1:14:25] Stepping pH = 6.17
[1:14:25] Dispensed 0.000141 mL of Acid (0.5 M HCl)
[1:14:30] Stepping pH = 6.07
[1:14:30] Dispensed 0.000024 mL of Acid (0.5 M HCl)
[1:14:36] Stepping pH = 6.06
[1:14:36] Dispensed 0.000024 mL of Acid (0.5 M HCl)
[1:14:41] Stepping pH = 6.06
[1:14:41] Dispensed 0.000094 mL of Acid (0.5 M HCl)
[1:14:46] Stepping pH = 5.98
[1:15:01] Stirrer speed set to 0

Sample name: **M08_octanol**   Experiment start time: **3/2/2018 8:29:22 PM**
Assay name: **pH-metric high logP**   Analyst: **Pion**
Assay ID: **18C-02009**   Instrument ID: **T312060**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02009_M08_octanol_pH-metric high logP.t3r**

Experiment Log (continued)

[1:15:24] Datapoint id 73 collected
[1:15:24] Charge balance equation is out by -45.5%
[1:15:24] Stirrer speed set to 60
[1:15:30] pH 5.98 -> 5.78
[1:15:30] Using cautious pH adjust
[1:15:30] Dispensed 0.000094 mL of Acid (0.5 M HCl)
[1:15:35] Stepping pH = 5.91
[1:15:35] Dispensed 0.000094 mL of Acid (0.5 M HCl)
[1:15:40] Stepping pH = 5.80
[1:15:40] Dispensed 0.000024 mL of Acid (0.5 M HCl)
[1:15:45] Stepping pH = 5.78
[1:16:00] Stirrer speed set to 0
[1:16:22] Datapoint id 74 collected
[1:16:22] Charge balance equation is out by -10.2%
[1:16:22] Stirrer speed set to 60
[1:16:27] pH 5.79 -> 5.59
[1:16:27] Using charge balance adjust
[1:16:27] Dispensed 0.000141 mL of Acid (0.5 M HCl)
[1:16:47] Stirrer speed set to 0
[1:17:11] Datapoint id 75 collected
[1:17:11] Charge balance equation is out by -22.3%
[1:17:11] Stirrer speed set to 60
[1:17:16] pH 5.58 -> 5.38
[1:17:16] Using cautious pH adjust
[1:17:16] Dispensed 0.000047 mL of Acid (0.5 M HCl)
[1:17:21] Stepping pH = 5.54
[1:17:21] Dispensed 0.000071 mL of Acid (0.5 M HCl)
[1:17:26] Stepping pH = 5.39
[1:17:42] Stirrer speed set to 0
[1:18:00] Datapoint id 76 collected
[1:18:00] Charge balance equation is out by -38.4%
[1:18:00] Stirrer speed set to 60
[1:18:05] pH 5.37 -> 5.17
[1:18:05] Using cautious pH adjust
[1:18:05] Dispensed 0.000024 mL of Acid (0.5 M HCl)
[1:18:10] Stepping pH = 5.38
[1:18:10] Dispensed 0.000165 mL of Acid (0.5 M HCl)
[1:18:15] Stepping pH = 4.87
[1:18:30] Stirrer speed set to 0
[1:18:53] Datapoint id 77 collected
[1:18:53] Charge balance equation is out by -202.4%
[1:18:53] Stirrer speed set to 60
[1:18:58] pH 4.81 -> 4.61
[1:18:58] Using cautious pH adjust
[1:18:58] Dispensed 0.000024 mL of Acid (0.5 M HCl)
[1:19:03] Stepping pH = 4.80
[1:19:03] Dispensed 0.000071 mL of Acid (0.5 M HCl)
[1:19:08] Stepping pH = 4.64
[1:19:08] Dispensed 0.000024 mL of Acid (0.5 M HCl)
[1:19:13] Stepping pH = 4.58
[1:19:28] Stirrer speed set to 0
[1:19:40] Datapoint id 78 collected
[1:19:40] Charge balance equation is out by -130.6%
[1:19:40] Stirrer speed set to 60
[1:19:45] pH 4.59 -> 4.39
[1:19:45] Using cautious pH adjust
[1:19:45] Dispensed 0.000047 mL of Acid (0.5 M HCl)
[1:19:50] Stepping pH = 4.52
[1:19:50] Dispensed 0.000047 mL of Acid (0.5 M HCl)

Sample name: **M08_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-02009**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02009_M08_octanol_pH-metric high logP.t3r**

Experiment start time: **3/2/2018 8:29:22 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[1:19:55] Stepping pH = 4.40
[1:20:10] Stirrer speed set to 0
[1:20:32] Datapoint id 79 collected
[1:20:32] Charge balance equation is out by -2.3%
[1:20:32] Stirrer speed set to 60
[1:20:37] pH 4.39 -> 4.19
[1:20:37] Using charge balance adjust
[1:20:37] Dispensed 0.000118 mL of Acid (0.5 M HCl)
[1:20:57] Stirrer speed set to 0
[1:21:08] Datapoint id 80 collected
[1:21:08] Charge balance equation is out by -19.7%
[1:21:08] Stirrer speed set to 60
[1:21:13] pH 4.22 -> 4.02
[1:21:13] Using cautious pH adjust
[1:21:13] Dispensed 0.000071 mL of Acid (0.5 M HCl)
[1:21:18] Stepping pH = 4.16
[1:21:18] Dispensed 0.000094 mL of Acid (0.5 M HCl)
[1:21:23] Stepping pH = 4.05
[1:21:23] Dispensed 0.000024 mL of Acid (0.5 M HCl)
[1:21:28] Stepping pH = 4.03
[1:21:28] Dispensed 0.000024 mL of Acid (0.5 M HCl)
[1:21:33] Stepping pH = 4.03
[1:21:34] Dispensed 0.000047 mL of Acid (0.5 M HCl)
[1:21:39] Stepping pH = 3.99
[1:21:54] Stirrer speed set to 0
[1:22:04] Datapoint id 81 collected
[1:22:04] Charge balance equation is out by -78.1%
[1:22:04] Stirrer speed set to 60
[1:22:09] pH 3.99 -> 3.79
[1:22:09] Using cautious pH adjust
[1:22:09] Dispensed 0.000141 mL of Acid (0.5 M HCl)
[1:22:14] Stepping pH = 3.88
[1:22:14] Dispensed 0.000094 mL of Acid (0.5 M HCl)
[1:22:19] Stepping pH = 3.82
[1:22:19] Dispensed 0.000047 mL of Acid (0.5 M HCl)
[1:22:24] Stepping pH = 3.80
[1:22:39] Stirrer speed set to 0
[1:22:50] Datapoint id 82 collected
[1:22:50] Charge balance equation is out by 0.9%
[1:22:50] Stirrer speed set to 60
[1:22:55] pH 3.80 -> 3.60
[1:22:55] Using charge balance adjust
[1:22:55] Dispensed 0.000423 mL of Acid (0.5 M HCl)
[1:23:15] Stirrer speed set to 0
[1:23:25] Datapoint id 83 collected
[1:23:25] Charge balance equation is out by 2.4%
[1:23:25] Stirrer speed set to 60
[1:23:31] pH 3.59 -> 3.39
[1:23:31] Using charge balance adjust
[1:23:31] Dispensed 0.000659 mL of Acid (0.5 M HCl)
[1:23:51] Stirrer speed set to 0
[1:24:09] Datapoint id 84 collected
[1:24:09] Charge balance equation is out by -5.5%
[1:24:09] Stirrer speed set to 60
[1:24:14] pH 3.41 -> 3.21
[1:24:14] Using charge balance adjust
[1:24:14] Dispensed 0.001035 mL of Acid (0.5 M HCl)
[1:24:34] Stirrer speed set to 0
[1:25:00] Datapoint id 85 collected

Sample name: **M08_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18C-02009**
Filename: **C:\Sirius_T3\Mehtap\20180302_exp29_logP_T3-2\18C-02009_M08_octanol_pH-metric high logP.t3r**

Experiment start time: **3/2/2018 8:29:22 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[1:25:00] Charge balance equation is out by -3.2%
[1:25:00] Stirrer speed set to 60
[1:25:05] pH 3.22 -> 3.02
[1:25:05] Using charge balance adjust
[1:25:05] Dispensed 0.001599 mL of Acid (0.5 M HCl)
[1:25:25] Stirrer speed set to 0
[1:25:36] Datapoint id 86 collected
[1:25:36] Charge balance equation is out by -5.0%
[1:25:36] Stirrer speed set to 60
[1:25:41] pH 3.03 -> 2.83
[1:25:41] Using charge balance adjust
[1:25:41] Dispensed 0.002422 mL of Acid (0.5 M HCl)
[1:26:01] Stirrer speed set to 0
[1:26:26] Datapoint id 87 collected
[1:26:26] Charge balance equation is out by -7.8%
[1:26:26] Stirrer speed set to 60
[1:26:32] pH 2.85 -> 2.65
[1:26:32] Using charge balance adjust
[1:26:32] Dispensed 0.003716 mL of Acid (0.5 M HCl)
[1:26:52] Stirrer speed set to 0
[1:27:02] Datapoint id 88 collected
[1:27:02] Charge balance equation is out by -9.4%
[1:27:02] Stirrer speed set to 60
[1:27:07] pH 2.68 -> 2.48
[1:27:07] Using charge balance adjust
[1:27:07] Dispensed 0.005621 mL of Acid (0.5 M HCl)
[1:27:27] Stirrer speed set to 0
[1:27:52] Datapoint id 89 collected
[1:27:52] Charge balance equation is out by 0.3%
[1:27:52] Stirrer speed set to 60
[1:27:57] pH 2.48 -> 2.28
[1:27:57] Using charge balance adjust
[1:27:58] Dispensed 0.008937 mL of Acid (0.5 M HCl)
[1:28:18] Stirrer speed set to 0
[1:28:31] Datapoint id 90 collected
[1:28:31] Charge balance equation is out by -2.8%
[1:28:31] Stirrer speed set to 60
[1:28:36] pH 2.29 -> 2.09
[1:28:36] Using charge balance adjust
[1:28:37] Dispensed 0.014087 mL of Acid (0.5 M HCl)
[1:28:57] Stirrer speed set to 0
[1:29:18] Datapoint id 91 collected
[1:29:18] Charge balance equation is out by -3.5%
[1:29:18] Stirrer speed set to 60
[1:29:23] pH 2.10 -> 1.95
[1:29:23] Using charge balance adjust
[1:29:23] Dispensed 0.016157 mL of Acid (0.5 M HCl)
[1:29:43] Stirrer speed set to 0
[1:30:03] Datapoint id 92 collected
[1:30:03] Charge balance equation is out by -25.8%
[1:30:03] Argon flow rate set to 0
[1:30:07] Titrator arm moved over Titration position